CONFERENCE PROCEEDINGS

Book of Abstracts

The 23rd International Symposium on Boron, Borides and Related Materials

ISBB 2026 – The 23rd International Symposium on Boron, Borides and Related Materials

University of California, Riverside, USA

August 30 - September 4, 2026

ISBB is a long-standing international forum with a history spanning more than six decades, dedicated to advancing discussions on the chemistry, physics, and materials science of boron, borides, and related materials. Since its inaugural meeting in New Jersey in 1959, the symposium has been held at venues worldwide, most recently in Paris (2022) and Istanbul (2024). We are delighted that ISBB is returning to the United States in 2026.

ISBB2026 will bring together leading scientists, engineers, and researchers from around the world to share recent progress, exchange ideas, and foster collaborations across disciplines. The scientific program will feature plenary and invited lectures, contributed oral presentations, and poster sessions, covering both fundamental research and emerging applications.

Located in Southern California, the University of California, Riverside offers a vibrant academic environment and convenient access to cultural, natural, and recreational attractions in the region.

We are grateful to the numerous participants, sponsors and volunteers (including undergraduate students) who have contributed to making this event a resounding success.

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Sunday	Welcome/registration + 2 memoriam talks from 3pm

Monday		**Tuesday**		**Wednesday**	
Structural Materials		Low Dimensional Materials 1		Magnetic and Quantum Materials 1	
8:30-9:00	Opening + Borax Talk	**8:30-9:05**	**Boris I. Yakobson**	**8:30-9:05**	**Jeff Snyder**
9.00-9.35	**Richard B. Kaner**	**9.05-9.40**	**Lai-Sheng Wang**	*9.05-9.30*	*Weiwei Xie*
9.35-10.00	*Jakoah Brgoch*	*9.40-10:05*	*Levan Chkhartishvili*	*9.30-9.55*	*Julia Zaikina*
10.00-10.15	Steven Smith	10.05-10.20	Osamu Oki	*9.55-10.20*	*Peter Franz Rogl*
10.15-10.50	**Sarah H. Tolbert**	10.20-10.35	Selcuk Acar	**10.20-10.40**	**Cofee break**
10.50-11.10	**Cofee break**	**10.35-10.55**	**Cofee break**	Magnetic and Quantum Materials 2	
Synthesis and Properties 1		Low Dimensional Materials 2		*10:40-11:05*	*Vladimir Antropov*
11.10-11.35	*David Portehault*	**10:55-11:30**	**E. D. Jemmis**	11.05-11.20	Shola Adeniji
11.35-12:00	*Susan Latturner*	11:30-11:45	Andrew J. Baublis	*11.20-11:45*	*Slavomir Gabani*
12:00-12:25	*Christina Birkel*	*11:45-12:10*	*Brandon Wood*	11:45-12:00	Karol Flachbart
12:25-1:45	**Lunch**	**12:10-1:30**	**Lunch**	*12:00-12:25*	*Sanjay Behura*
Catalysts and Electrocatalysts 1		Synthesis and Properties 2		**12:25-1:45**	**Lunch**
1:45-2:10	*Yuri Grin*	**1:30-2:05**	***Hanno zur Loye***		
2:10-2:35	*Edward Gillan*	*2:05-2:30*	*Takahiro Kondo*		
2:35-2:50	Klaudia Zielinkiewicz	*2:30-2:55*	*Özge Balci Çagiran*		
2:50-3:15	*Georgiy Akopov*	2.55-3.15	Poster flash-talks		
3:15-3:35	**Cofee break**	**3:15-3:35**	**Cofee break**		
3.35-3.55	Poster flash-talks	Complex Structures			
Catalysts and Electrocatalysts 2		*3:35-4:00*	*Kaoru KIMURA*		
3:55-4:20	*Richard G. Blair*	*4:00-4:25*	*Kohei SOGA*		
4:20-4:45	*Kabeer Jasuja*	4:25-4:40	Kunio Yubuta		
4.45-5.00	Paul Oftedahl	*4:40-5:05*	*Wanlu Li*		
5:00-5:25	*Michael T. Yeung*	*5:05-5:30*	*Tadashi Ogitsu*		
5:25-5:40	Shohei Shimozato				
6:00-7.00	Poster Session 1	6:00-7.00	Poster Session 2		

Thursday

B-N and Related Materials 1

8:30-9:05	**Zhifeng Ren**
9.05-9.30	*Xi Chen*
9.30-9.55	*Aaron J. Rossini*
9.55-10.30	**Angel A. Martí**
10.30-10.45	Zhenguo Huang
10.45-11.05	**Cofee break**

B-N and Related Materials 2

11.05-11.30	*Hongxing Jiang*
11.30-11:55	*Richard Wilson*
11:55-12:20	*Jianlin Liu*
12:20-1:40	**Lunch**

Molecular and Organoboron Compounds 1

1:40-2:15	**Francois Gabbai**
2:15-2:50	**Frieder Jaekle**
2:50-3:05	Subir Maji
3:05-3:30	*Dmitry Peryshkov*
3:30-3:50	**Coffee break**

Molecular and Organoboron Compounds 2 (Frieder Jaekle)

3:50-4:15	*Hosea Nelson*
4:15-4:40	*Matt Conley*
4:40-5:15	**Don Tilley**
5:15-5:40	*Joshua Figueroa*

6:00-7:00	Transfer
7:00 - ?	Galla Dinner

Friday

Physical Properties and Applications 1

8:30-9:05	**Iwao Matsuda**
9.05-9.30	*Takao Mori*
9.30-9.55	*Nathalie Vast*
9.55-10.20	*Mahesh Neupane*
10.20-10.40	**Cofee break**

Physical Properties and Applications 2

10:40-11:05	*Anastassia N. Alexandrova*
11:05-11:20	Naoki Uemura
11:20-11:35	Natsumi Noguchi
11:35-11:50	Keita Sasaki
11:50-12:05	**Closing remarks**
12:05	**Lunch + Departure**

SECTION 01

Plenary Speakers

Conference section divider

Superhard Metal Borides

J. Keane[1], S.G. Hamilton[1], C.L. Turner[1], Y. Han[1], M.A. Huizar[1], S.H. Tolbert[2] and R.B. Kaner[2*]

[1]Department of Chemistry and Biochemistry, University of California, Los Angeles (UCLA)

[2]Department of Chemistry and Biochemistry, Department of Materials Science and Engineering, and California NanoSystems Institute (CNSI), University of California, Los Angeles (UCLA)

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The increasing demand for high-performance cutting and forming tools, along with the shortcomings of traditional tool materials such as diamond (unable to cut ferrous materials), cubic boron nitride (expensive) and tungsten carbide (relatively-low hardness), has motivated the search for new superhard materials for these applications. This has led us to a new class of superhard materials, dense refractory transition-metal borides, which promise to address some of the existing problems of conventional superhard materials. For example, we have synthesized rhenium diboride (ReB_2) using arc melting at ambient pressure.[1] This superhard material has demonstrated an excellent electrical conductivity and superior mechanical properties, including a Vickers hardness of 48.0 GPa (under an applied load of 0.49 N) and the ability to scratch diamond. To further increase the hardness and lower the materials costs, we are exploring high boron content metal borides including tungsten tetraboride (WB_4).[2] We have synthesized WB_4 by arc melting and studied its hardness and high-pressure behavior. With a similar Vickers hardness (43.3 GPa under a load of 0.49 N) and bulk modulus (326-339 GPa) to ReB_2, WB_4 offers a lower cost alternative and has the potential to be used in cutting tools. To further enhance the hardness of this superhard metal, we have created binary and ternary solid solutions of WB_4 with Cr, Mn and Ta, the results of which show a hardness increase of up to ~20%.[3,4] As with other metals, these metallic borides can be readily cut and shaped using electric discharge machining (EDM).

References

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[2] Pangilinan, L.E.; Hu, S.; Hamilton, S.G.; Tolbert, S.H.; Kaner, R.B. Hardening Effects in Superhard Transition-Metal Borides. *Accounts of Materials Research*, 2022, *3*, 100-109.

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Tuning the Mechanical Properties of Transition Metal Borides Through Control of Atomic and Nanoscale Structure

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In this talk, we will examine a family of super-hard materials based on late transition metal borides. These materials are exciting because, unlike conventional superhard materials diamond and cubic boron nitride, they can be synthesized at atmospheric pressure. The materials were initially constructed using three very simple molecular design rules: 1) use late transition metals to create high electron density so that the materials are incompressible; 2) add boron to build strong covalent bond to prevent slip and generate hard materials; 3) use solid-solution effects to further tune materials properties. In this talk, we will combine these ideas with materials synthesis, indentation hardness measurements, and high-pressure diffraction to gain an understanding of how the hardness can be tuned using chemical composition and bonding motifs. To gain a global understanding of the family of materials we will consider a broad range of crystal structures including metal (M) diborides (MB_2), tetraborides (MB_4), and dodecaborides (MB_{12}), as shown below. Our results show that crystal structure control, metal atom composition, and small element hetero-atom doping are all effective routes to improve hardness.[1] We will then consider a new design rule: 4) use nanoscale architecture to further enhance hardness through the Hall-Petch effect in metal boride nanocrystals.[2] Here, novel synthetic methods are required to make materials, and remarkable changes in mechanical properties can be achieved using control of nanoscale architecture.

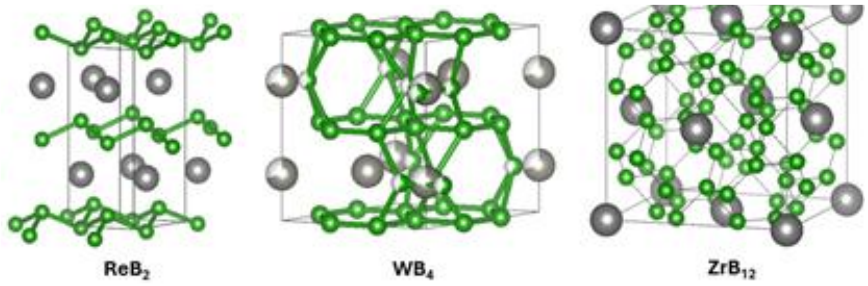

Fig. 1. Crystal structures of ReB_2, WB_4, and ZrB_{12}. Green atoms represent boron while gray atoms represent metals.

References

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From Boron Buckyball to 2D Borophene and Borides: A Theory Perspective

Boris I. Yakobson, Evgeni Penev*
Rice University, Houston, Texas
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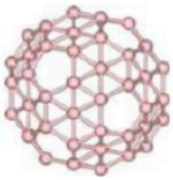
This talk traces theoretical developments that helped define and interpret boron nanostructures. The B_{80} fullerene,[1] predicted in 2007 (and recently confirmed by L.-S. Wang's experiments, *Chemical Science*, 2026, DOI: 10.1039/D6SC02674E), soon even reached popularity of the High School Olympics (Panel 1). It pointed toward stable low-dimensional architectures beyond known 3D bulk allotropes. Extending this logic (by "infolding the buckyball", Panel 2) to the 2D showed that boron does not simply mimic graphene. Stable monolayers instead arise from vacancy-patterned triangular networks, producing a family of borophene polymorphs[2] that became central to the field. Theory then addressed the key synthetic challenge:[3] how can such sheets be realized experimentally? Calculations showed that specific metal substrates can stabilize selected borophene phases, suggesting growth routes later validated by synthesis on Ag and Au surfaces. These materials stimulated further studies of borophene's anisotropic electronic structure, mechanics, possible superconductivity.[4] Recent work has expanded beyond monolayer borophene, to multilayer growth and the strong substrate-interactions, where B on metals forms nanolayer borides[5] (Panel 3) rather than chemically distinct borophene. Examples show how first-principles theory connects bonding, structural prediction, substrate selection, and emergent properties in low-dimensional boron materials.

第五届"我爱奥赛杯"高中化学竞赛试题

第 1 题（6 分）硼的化学丰富多彩，也是材料化学研究的热点之一。

1-1、最近美国 Rice University 的教授 Boris Yakobson 与其同事预测了一种硼巴基球(B_n，如图所示)的存在，这种分子组成与 C_{60} 相似，但在它每个六边形的中心有一个额外的原子，显著提高了其稳定性。

则 n=_____



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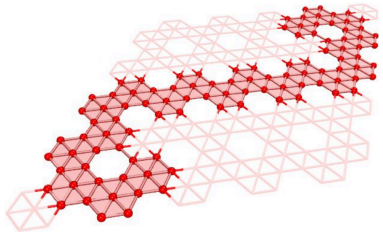

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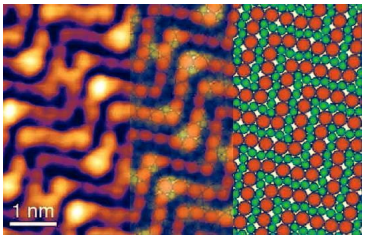

3

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Boron Nanoclusters

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The study of carbon clusters led to the discoveries of fullerenes, carbon nanotubes, and graphene. Are there other elements that can form similar nanostructures? Motivated by this question, we have been investigating the size-dependent structures and chemical bonding of boron nanoclusters using photoelectron spectroscopy and theoretical calculations [1, 2]. We have found that bare boron clusters possess planar structures [3], in contrast to that of bulk boron, which is dominated by three-dimensional polyhedral building blocks. The discovery of planar boron clusters laid the foundation for 2D boron nanomaterials [4]. In particular, the observation of the planar B_{36} cluster with a central hexagonal vacancy provided the first experimental evidence that borophene was viable (Fig. 1) [5]. Borophene has been synthesized and characterized on inert substrates, forming a new class of synthetic 2D materials [6]. The B_{40} cluster was the first confirmed all-boron fullerene [7], which possesses D_{2d} symmetry with a cage diameter slightly smaller than that of C_{60}. In this talk, I will review progresses and focus on recent advances in the investigation of large boron clusters, including 2D-3D transitions, the appearance of bulk-like boron features [8], and other novel boron nanostructures.

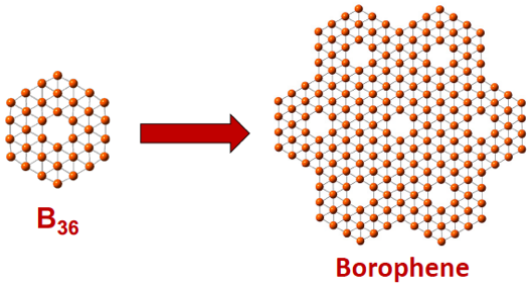

Fig. 1. From planar boron clusters to borophene.

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A Structural Chemistry for Boron

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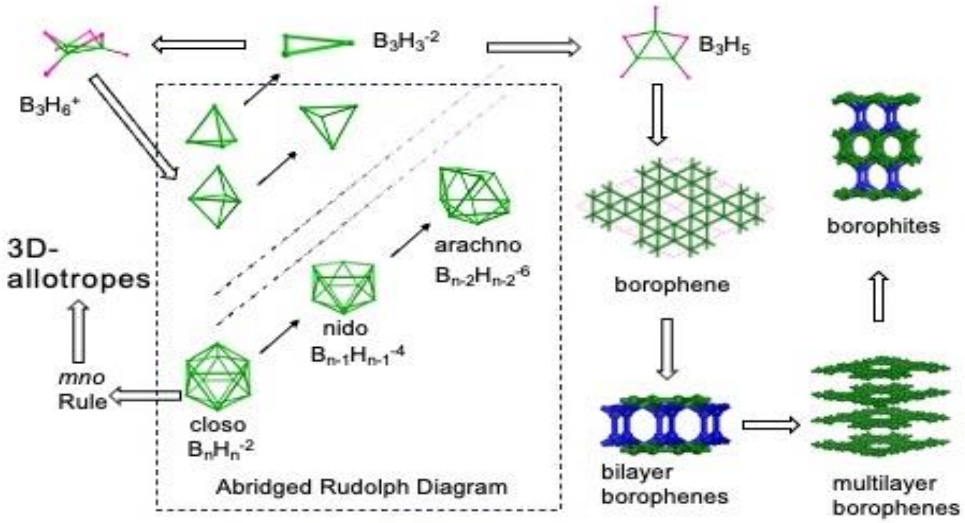
In comparison to the chemistry of carbon, that of boron is only evolving: the relationship between polyhedral boranes, 3D allotropes, 2D allotropes (Borophenes and Borophites) and boron clusters are not well understood. We have attempted to "understand" the structural chemistry of boron through three membered rings and an extended Rudolph diagram.[1] Electronic structure of MgB2 helps in this process. Many boron-rich metal borides,borospherenes and small boron clusters can be brought under this structural paradigme; yet much remains to be understood.[2,3]



Extended Rudolph Diagram

Acknowledgements: Members of the group, past and present, are thanked for converting my vague thoughts to definite ideas. Collaboration with Prof. Sundargopal Ghosh and funding through National Science Chair-ANRF, India, are much appriciated.

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[3] E.D. Jemmis et al To be published.

Boron Chalcogen Mixture Method and/or Flux Crystal Growth: Intentional and Unintentional Syntheses of Borates

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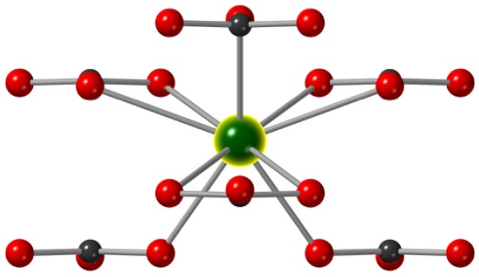
The zur Loye group has used the Boron Chalcogen Mixture (BCM) method for several years to synthesize oxygen free sulfides. Elemental boron can react with oxygen to form B_2O_3, a facile product that can be removed by dissolving it in water or methanol. This approach enables us to start with oxide reagents and end up with pure sulfides, chalcogenides, or tellurides. Initially developed for use with actinides, mostly uranium and thorium, we have extended its use to rare earth oxides, transition metal oxides, and main group oxides.

In this presentation the BCM method will be discussed and illustrated how it can be used for the synthesis of new chalcogenides. Importantly, we can couple this reaction with fluxes and grow high quality chalcogenide single crystals. In several instances the boron is incorporated into the product. For example, the synthesis of B12-cluster containing selenoborate, $Na_2B_{12}Si_6Se_{18}$, resulted when a reaction to target $CaEuUSi_2Se_8$ was performed, and under certain conditions it is possible to prepare thioborates, such as $LnBS_3$ (Ln = La, Ce, Pr, Nd) and $(Nd_3SiS_7)_2(Nd_3SiS_4BS_3)$.

The zur Loye group has also explored borates via high temperature flux single crystal growth to target actinide containing materials. This approach has proven very useful and resulted in the formation of numerous borates, including $AmBO_3$,[1] $Ba_3Am_2(BO_3)_4$, $Ca_5Am(BO_3)_4Cl$, $Na_2(PuO_2)(BO_3)$, $Na_2(UO_2)(BO_3)$, $A_3Ln(BO_3)_2$ (A = Na, K; Ln = lanthanide), SrB_2O_4, and $A_2(UO_2)B_2O_5$ (A = Cs, Rb, K). A variant of a flux, an ionic liquid, was also used and resulted in a novel americium borate cluster, $Am_4B_{22}O_{42}Cl_{12}$, and several lanthanide analogs, $Ln_4B_{22}O_{42}Cl_{12}$ (Ln = Ce, La, Nd).



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The Possibility of New Complex Magnet Materials

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Magnets are essential for mobile consumer electronics, electric motors that power industry and the future of transportation as well as generating and transforming most electric power. Strong magnets reduce the size and weight of motors and generators as well as improve efficiency. The most powerful $Nd_2Fe_{14}B$-based magnets have a complex structure like millions that are expected to exist but have not been made and characterized. With the recent developments of AI materials discovery techniques, which enable data-driven and machine-learning-assisted screening, together with computational approaches that can accurately predict intrinsic magnetic properties of a given structure, and high-throughput autonomous labs, the discovery of new, ultra-powerful magnet materials is now quite possible.

What Is Unknown of Boron Arsenide?

Zhifeng Ren

Department of Physics and

Texas Center for Superconductivity at the University of Houston

Ultrahigh thermal conductivity in boron arsenide (BAs) was first predicted in 2013 by David Broido and colleagues using first-principles calculations, suggesting values comparable to that of diamond. This prediction was subsequently verified experimentally during the 2015–2018 period. Since then, it has also been discovered that BAs exhibits ultrahigh carrier mobility, a property highly desirable for advanced applications, particularly in high-power electronics.

By 2018, thermal conductivity values of approximately 1300 $W \cdot m^{-1} \cdot K^{-1}$ were experimentally achieved, in good agreement with theoretical predictions. However, with continued improvements in single-crystal growth techniques, thermal conductivity exceeding 2000 $W \cdot m^{-1} \cdot K^{-1}$ was observed in 2025. These values surpass current theoretical limits and cannot be explained by existing models, raising a fundamental question: what is the ultimate thermal conductivity of BAs?

In this talk, I will present both the established understanding and the remaining open questions in the study of boron arsenide single crystals.

Fluorination of Boron-Nitride Nanotubes

*Alina Chow,[1] Kexin Ling,[1] Benjamin A. Atterberry,[3] Ying Chen,[1] Dmitri V. Kosynkin,[2] Matteo Pasquali,[2] Aaron J. Rossini,[3] Angel A. Martí[1]**

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Boron nitride nanotubes (BNNTs) are tubular nanostructures that could be used as building blocks for advanced macroscopic materials, thanks to their exceptional thermal, mechanical, and electronic properties. Yet, their inherent chemical inertness presents a significant challenge to tuning their properties for large-scale processing. Unlocking the full potential of BNNTs hinges on a deeper understanding and control of their surface chemistry. Here we report on a novel, room-temperature fluorination procedure for BNNTs using hydrofluoric acid (HF). This mild method achieves a high fluoride content (up to ~3.7 wt%), which was confirmed to be chemically bonded to the boron sites through comprehensive spectroscopic and thermal analysis. We also studied the conductivity and bandgap of BNNTs and observed that fluorinated BNNTs present unique photophysical properties that are reversible upon defluorination. Thus, BNNT fluorination represents a facile synthetic strategy to modulate the properties of BNNTs.

Tellurium-based strategies for the transport of ions across biological membrane mimics

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Over the past two decades, we have developed a series of cationic main group Lewis acids which can be used as sensors for anions in water. By studying a series of boron derivatives bearing pendant sulfonium or telluronium moieties, we realized that the group 16 element could engage favorably with the anionic guest via sigma hole interactions. In this presentation, we will report on the latest results we have obtained in this line of study. We will also disclose our recent findings concerning the use of tellurium-containing derivatives for the transport of anions across phospholipid bilayers. In particular, we will show that telluronium cations readily interact with anions via chalcogen bonding interactions, leading to distinct anion transport properties that we have characterized using phospholipid-based vesicle assays. We will also demonstrate that the redox activity of the group 16 element can be harnessed for the design of stimuli-responsive transporters, which can be activated by simple biological redox regulators, such as glutathione. Although our work has focused on anions, the last part of this presentation will show how redox-controlled and redox-switchable intramolecular N-Te chalcogen bonding can be leveraged for the stimuli-responsive transport of biologically relevant divalent metal ions.

B-N Doped Molecular and Polymeric Materials

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The incorporation of main group elements into molecular and polymeric materials is frequently exploited to achieve unusual properties and to enable new functions.[1] For instance, tricoordinate boron's participation in pi-delocalization can have a dramatic effect on the optical properties by selectively lowering the LUMO orbital levels.[2] The electron-deficient character of boron also enables dynamic Lewis acid-base interactions, which trigger strong perturbations of the electronic structure and enable assembly of novel supramolecular materials.

Our group has developed versatile approaches for incorporating borane Lewis acids and Lewis pairs into conjugated molecular, macrocyclic and polymeric materials with a view at potential applications in organic electronics, sensing, (photo)catalysis, bioimaging, and therapeutics.[3-4] Furthermore, we have pioneered the selective attachment of boranes and azaborines to polyolefins through direct polymerization and post-polymerization approaches.[5]

These polymers are finding applications as supported catalysts and as building blocks of dynamic polymer networks. In this talk, I will discuss some of our recent discoveries, highlighting the effect of B-N functionalization on the material properties and the impact in diverse application fields.

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Metal-Mediated Ring Fusions for Introduction of Antiaromatic Rings, including Boroles, into Conjugated Nanocarbons

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Graphene and its properties have motivated research on large polycyclic aromatic hydrocarbons (PAHs), which are basic building blocks of graphene and other carbon-rich nanostructures. Various PAHs are of interest as molecular models, synthetic precursors, and components in electronic devices, due to unique properties that result from their extended conjugation and rigidity. A central goal in this area is the synthetic manipulation of electronic properties for nanocarbon materials, by generation of well-defined dimensionalities and functionalizations. We have employed selective metal-mediated cycloadditions for extension of π systems and introduction of multiple fused rings in the synthesis of π-conjugated oligomers, polymers, and macrocycles, mainly *via* the reductive coupling of alkynes with a low-valent zirconocene reagent. Boroles are a 4π-electron antiaromatic system, usually stabilized electronically by benzene ring fusion or sterically by substitution with aryl species. Here, zirconium boron transfer is used to generate a series of phenanthrene fused multi-boroles. These boroles are strongly colored and exhibit long absorption onsets, which is indicative of their high antiaromatic character. In particular, an [11]-expanded helicene tris-borole is generated to study the interplay of chirality and antiaromaticity.

Exploring 2D boron materials

by experimental robots and machine learning analyses

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Two-dimensional (2D) boron materials have been intriguing playgrounds to examine low-dimenaional physics and promising platforms to develop funcional chemistry [1-6]. For the material characterizations, X-ray spectroscopy has been a powerful method since it quantitatively evaluates chemical components and directly probes electron states of a sample. Recently, we have combined such an X-ray spectroscopy technique with automated robot controls and with spectral analyses using machine learning at the synchrotron radiation beamline, NanoTerasu BL08U [7-9]. Using the system, we carried out demonstraion experiments on 2D boron materials, such as h-BN and HB sheets. We have succeeded in indentifying unknown samples and in discovering unidentified materials in a high-throughput way. In addition, we found that the analyzed data carry information on defects and film thickness that charaterize individuality of the sample. In the present talk, I will introduce the system in detail and discuss its future usages for boron science.

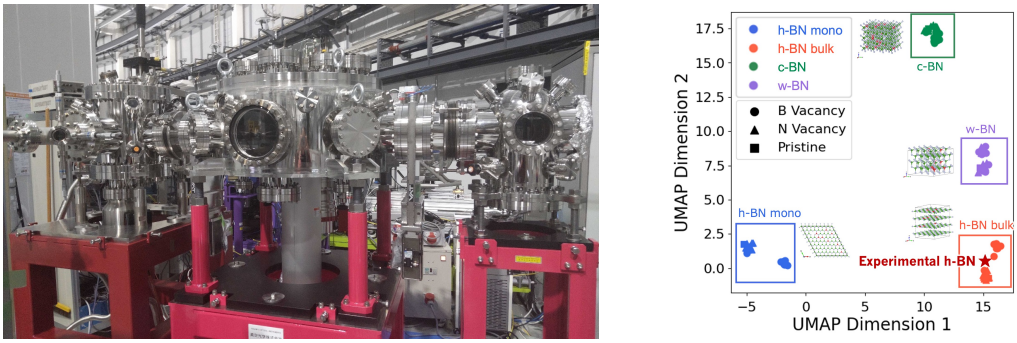

Figure (left) The high-throughput X-ray spectroscopy system at the synchrotron radiation beamline, NanoTerasu BL08U. (right) Spectral analysis of the machine learning (UMAP) [8].

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SECTION 01

Invited Speakers

Conference section divider

Visible Light Driven C–C and C–H Bond Activation over Boron-Rich Solids

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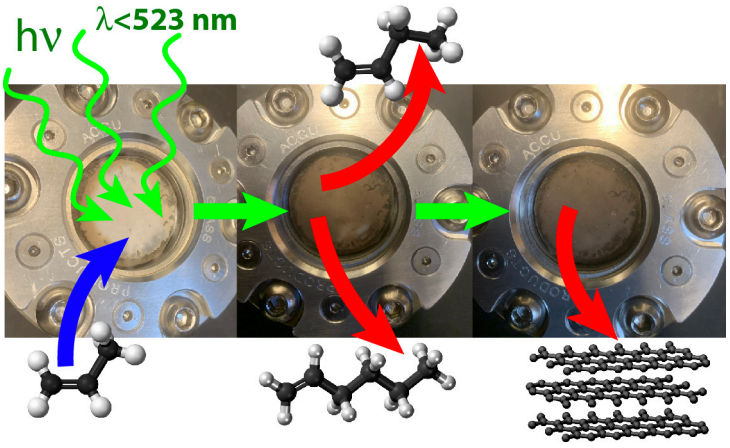
Direct conversion of hydrocarbons into value-added carbon materials under mild conditions represents a significant challenge in catalysis and materials chemistry. Presented here is a room temperature, visible-light-driven photocatalytic approach based on metal-free boron-rich materials. Rapid dehydrogenation of propene to carbon was observed under ambient conditions. Boron-rich catalytic materials were prepared through two complementary approaches: generation of nitrogen vacancies (V_N) in hexagonal boron nitride (*dh*-BN) and a top-down chemical etching process applied to AlB_2 to produce bulk quantities of two-dimensional boron sheets consisting predominantly of boron α′ phases. This process provides a practical and scalable pathway toward production of this emerging two-dimensional boron material. Under visible-light illumination, these boron-rich materials promote C–H and C–C bond activation, resulting in the formation of C_4–C_6 intermediates and ultimately graphitic carbon. Focused laser illumination was additionally used to pattern carbon formation and produce carbon microstructures with aspect ratios approaching 500 within seconds to minutes.[2] These reactions occur under ambient conditions without metal-based catalysts and demonstrate the potential of boron-rich photocatalytic systems as a new platform for hydrocarbon valorization, carbon materials synthesis, and development of next-generation photocatalysts for hydrocarbon conversion chemistry.



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Learning Stabilizing Motifs in Amorphous Materials: Boron-Induced Short-Range Order

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Amorphous materials lack long-range order, yet their stability and functionality are governed by underlying short-range order (SRO) motifs that remain poorly understood and difficult to control. Identifying the key structural features that stabilize disordered networks is therefore a central challenge in materials design.

In this talk, I will present a unifying perspective in which boron acts as a critical stabilizing element that induces distinct short-range order in amorphous materials. Owing to its electron-deficient nature and ability to form multi-center bonds, boron promotes the formation of locally preferred structural motifs (e.g., BOx units and network-forming clusters) that suppress crystallization, enhance structural homogeneity, and lower the energy landscape of disordered systems.

To systematically uncover and quantify these effects, we developed ApolloX, a physics-informed generative modeling framework that incorporates explicit SRO constraints into structure generation. By encoding local chemical environments and coordination statistics, ApolloX efficiently explores the configurational space of amorphous materials and identifies energetically favorable structures consistent with experimental observables.

Our results show that boron incorporation leads to narrower energy distributions, enhanced glass-forming ability, and improved agreement with experimental signatures such as pair distribution functions (PDF) and X-ray absorption spectra (XAS). More importantly, the framework reveals that boron-induced SRO is not merely a compositional effect, but a transferable structural principle that governs stability across a wide range of multi-element and high-entropy amorphous systems.

This work establishes short-range order engineering, guided by boron chemistry, as a general design strategy for stabilizing amorphous materials, and highlights how physics-informed generative models can bridge atomic-scale understanding with predictive materials discovery.

Y(*TM*)B_4 Catalysts: From Water Splitting to Reforming Reactions

Professor Georgiy Akopov, Rutgers University, Newark

Metal borides are good catalysts for a variety of catalytic processes. Borides containing Mo and Ni-Fe are stable and efficient catalysts for water splitting reactions (HER and OER). Fe, Co and Ni borides are efficient catalysts for hydrolysis and nitrogen reduction reactions. Furthermore, metal borides (Co and Ru-Sn) as well as boron carbide ("B_4C") can perform a variety of hydrogenation (fatty acid esters to alcohols) and dehydrogenation (propane and methanol) reactions. Layered ternary metal borides, $YCrB_4$, $YMoB_4$, and YWB_4 (*Pbam*) were analyzed as hydrogen evolution reaction (HER) eletrocatalysts. YWB_4 demonstrated the highest catalytic activity, surpassing the Pt/C catalyst by 185 mV overpotential at an industrially relevant current density of 1000 mA/cm^2. Stability testing revealed that YWB_4 retained 95% of its initial activity after 25 hours of continuous operation (5000 cycles) at 1000 mA/cm^2, underscoring its potential as a robust and sustainable HER catalyst for hydrogen production. $YNiB_4$ (*I*4/*mmm*) was analyzed for its ability to perform hydrogenation reaction. Preliminary results show promising activity for WO_3 hydrogentation. $YNiB_4$ furthermore showed good HER activity (surpassing Ni_2B).

Spin Defects in Hexagonal Boron Nitride for Quantum Information Science

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Associate Faculty of Computational Science Research Center
San Diego State University

Faculty Researcher, MonArk NSF Quantum Foundry

Abstract:
Hexagonal boron nitride (hBN), a two-dimensional wide-bandgap van der Waals insulator, has emerged as a promising solid-state platform for quantum information science due to its ability to host optically addressable spin defects stable at room temperature. These defect centers introduce localized electronic states within the bandgap with spin-dependent optical transitions, enabling applications in quantum-enhanced sensing and quantum communication. However, scalable deployment is hindered by the lack of deterministic defect engineering in wafer-scale hBN, limited quantum emission efficiency, and short spin coherence times driven by environmental decoherence and material inhomogeneity.

In this talk, I will present our group's efforts to overcome these challenges through a combined approach of deterministic defect engineering, cavity quantum electrodynamics, and coherent spin control. We demonstrate generation of spin defects in wafer-scale hBN with high spectral purity, strongly polarized emission, and robust photostability. Integration with nanophotonic cavities enables exploration of the cavity–defect coupling regime, including Purcell-enhanced emission and modified radiative dynamics toward cooperative light–matter interaction. In addition, I will discuss emerging approaches for coherent spin manipulation and spin–photon interfacing, targeting improved initialization, readout fidelity, and coherence.

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Simulations of superionic solid electrolytes based on boron clusters

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Metal hydroborates can exhibit extraordinary ionic conductivity and good electrochemical stability, making them attractive as novel solid electrolytes for next-generation lithium and sodium batteries. In addition, these materials also present wide tunability in structure and composition, making them an excellent platform for exploring underlying mechanisms and developing new descriptors for ion conduction. I will show how extensive computational diffusion simulations have been applied to closo-borates in order to systematically isolate key chemical and structural factors that determine ionic conductivity. The results highlight key connections between local frustration, dynamic correlation, and ionic mobility, connected to the specific geometry and electronic structure of the boron-based clusters. Different classes of frustration present in hydroborates will be presented, arising from factors such as off-stoichiometry, competition between interstitial site occupancies, symmetry incompatibilities between local bonding character and lattice geometry, and dynamical frustration coupled to anharmonic processes. The relevance of these factors for cation mobility will be discussed, with a view towards developing design rules for engineering faster room-temperature ionic conductors based on hydroborate salts.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Formation of dynamic charge stripes in quantum magnet TmB_4

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Intermetallic binary boron compounds are modeling systems for the study of superconductors (MgB_2, YB_6, ZrB_{12}, LuB_{12}), topological Kondo insulators (SmB_6, YbB_6, YbB_{12}), heavy fermion or amplitude-modulated antiferromagnets (CeB_6, HoB_{12}), as well as quantum magnets (TmB_4, HoB_4) [1]. The origin of charge transport, specific heat and magnetization anisotropy has been explained in some of them by the observation of dynamic charge stripes (nanoscale electronic instabilities) [1, 2]. The metallic tetraboride TmB_4 is one of the best-known representatives of the 2D frustrated Shastry-Sutherland lattice (SSL). The long-range Ruderman-Kittel-Kasuya-Yosida exchange interaction between magnetic moments leads to antiferromagnetic ordering of dimers. The crystal field effect at Tm^{3+} ion sites leads to strong Ising anisotropy along the [001] axis, thus allowing the manifestation of the SSL in the {001} planes. To visualize the dynamic charge stripes in TmB_4, a precise X-ray diffraction study has been carried out for the first time at 30 K (Figure). The obtained results are discussed and compared with those on other magnetic borides.

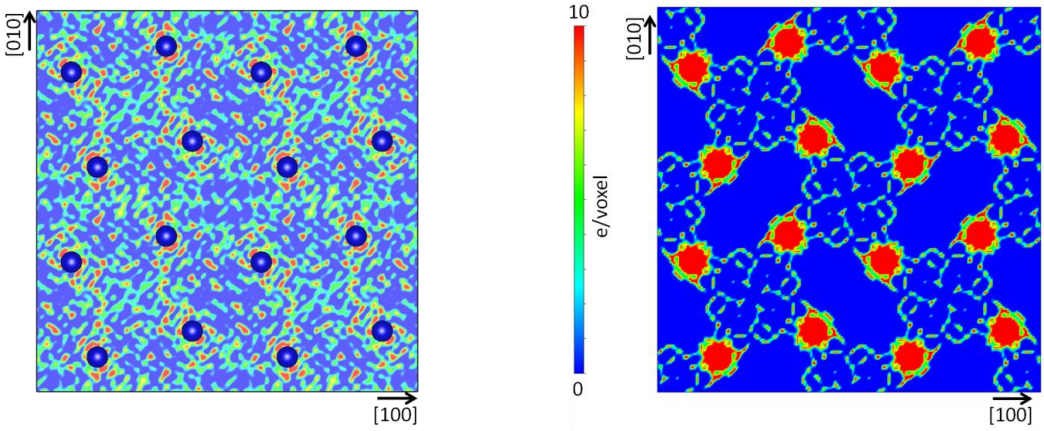

Figure: Electron density distribution obtained using diference Fourier synthesis (left) and maximum entropy method (right) in the (001) plane of TmB_4 crystal structure in a 2x2 unit cell at 30 K. Electron density peaks are cut off on the level of 5 e/A^3 and 10 e/voxel respectively (blue spheres on the left and red spots on the right show the positions of thulium atoms).

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β-Rhombohedral Boron – A Mysterious Single-Element Solid –

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Since the report by Sands and Hoard in 1957 of a β-rhombohedral boron structure containing approximately 108 atoms per unit cell, the crystal structure of β-boron has been intensively studied. Subsequent investigations have established a model based on a B_{105} framework with partial occupation of the B16 sites and partial vacancy of the B13 sites, leading to the now-standard B106.5 structural model. It is widely accepted that the electrical conduction near room temperature is governed by Motts variable-range hopping (VRH) mechanism, in which intrinsic acceptor levels associated with the occupation of the B16 sites are believed to play a crucial role [1, 2].

Despite this apparent consensus, several long-standing puzzles remain unresolved. First, even experiments conducted on highly pure samples report a remarkably large scatter in the lattice volume. Second, both the electrical conductivity and its temperature dependence exhibit a distinct change around 550 K. Third, light irradiation has been found to induce changes in the lattice volume. Furthermore, recent studies have suggested that hydrogen may be involved in these structural changes [3, 4, 5].

In this work, we focus on the occupation of the B16 sites and the incorporation and release of hydrogen, as well as the effects of heat and light and their relation to intrinsic acceptor levels. On this basis, we discuss key experimental issues that should be addressed in future studies to achieve a comprehensive understanding of β-rhombohedral boron.

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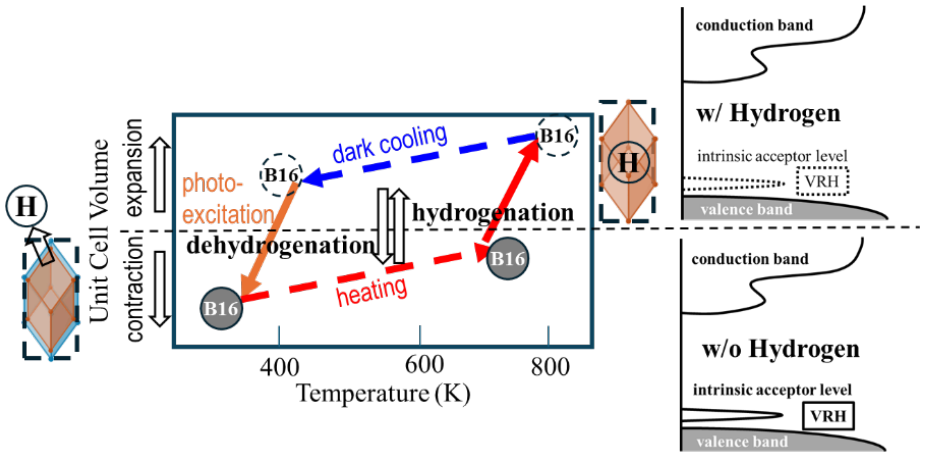

Figure. Overview of structural and physical property changes in β-B accompanied by hydrogen incorporation and release (lattice volume, B16 site occupancy, intrinsic acceptor level and electrical conduction mechanism).

Role of B and Al in Structural Stability and Magnetic Behavior

Weiwei Xie

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Boron and aluminum play critical roles in stabilizing crystal structures and tuning electronic and magnetic properties in intermetallic compounds. In this presentation, I will discuss two representative examples illustrating how light p-block elements influence structural stability and emergent physical behavior. In the first study, high-pressure single-crystal X-ray diffraction and electrical resistance measurements on $SmRh_3B_2$ reveal an unusual pressure-driven structural transition, demonstrating the important role of boron in maintaining structural integrity under extreme conditions. In the second study, temperature-dependent single-crystal X-ray diffraction and anisotropic magnetic susceptibility measurements on a uranium-based intermetallic compound uncover a subtle temperature-driven isosymmetric structural transition without crystallographic symmetry breaking. Distinct anomalies are observed in the lattice parameters, U-Al bond distances, and anisotropic displacement parameters near the transition region, accompanied by strong field-direction-dependent magnetic susceptibility. These results suggest pronounced magnetoelastic coupling between the lattice and U 5f electronic states, highlighting how subtle rearrangements of the local bonding environment involving Al can strongly influence anisotropic magnetic behavior. Together, these studies demonstrate the essential roles of B and Al in controlling structural stability, bonding, and correlated electronic phenomena in complex intermetallic materials.

Investigation of the Optimal Boron Content in Master Alloys Produced by SHS-Metallurgy from Industrial Wastes

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Complex master alloys based on the Fe–Mn–B system were produced using cost-effective and environmentally friendly SHS metallurgy technology (Self-propagating High-temperature Synthesis). To reduce the cost of the SHS master alloys, iron-containing waste and oxides of the elements involved in the synthesis were utilized. Aluminum powder served as the metal-reducing agent, which was replaced by aluminum shavings in amounts of up to 20%. The experiments were conducted using SHS metallurgy techniques in a laboratory high-pressure reactor and a centrifugal machine. The research objectives were successfully achieved using the laboratory centrifugal setup.

During the production of the SHS master alloys, the synthesis patterns were identified, and the chemical composition and properties of the resulting materials were established. Furthermore, the optimal boron content for producing a low-melting master alloy was determined. Sufficient quantities of boron-containing master alloys were produced for the alloying of steel and cast iron. Research has established the optimal and required amount of boron for alloying iron-based alloys. It was found that the amount of boron-containing master alloy required for cast iron is an order of magnitude higher than that for steel. To enhance the physical and mechanical properties of the iron-based alloys, appropriate heat treatment was performed. The microstructure and properties of the resulting iron alloys were subsequently investigated.

Synthesis and thermoelectric & other properties of bulk metal higher borides

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[2]Graduate School of Pure and Applied Sciences, University of Tsukuba
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Thermoelectric materials are recently of increasing interest for low-grade waste-heat energy harvesting [1] and as IoT power sources [2]. High temperature materials like borides can also be of interest for specialized applications [3] like topping cycles of power plants and RTGs [4]. Metal higher borides with cluster structures and interesting internal symmetries tend to have intrinsic low thermal conductivity despite strong bonding and intrinsic high sound velocity [5]. Large Seebeck coefficents and p- and n- type control have also been achieved for some prospective high temperature thermoelectric metal higher borides. Synthesis of metal higher borides are typically difficult, and I will make overview and also present recent advancements in bulk synthesis methods. For many of the novel metal boride phases which do not melt stably, it is necessary to utilize sintering methods, such as the borothermal reduction method which can utilize inexpensive metal oxide raw materials. Recently, methods like reactive spark plasma sintering (RSPS), liquid phase sintering, and gas/solid reaction, have yielded radically accelerated synthesis of some novel metal borides, and details and guidelines for future will be presented. Often dependence on synthesis methods for various properties like hardness, thermal conductivity have been observed, and I will also give a recent systematic study we carried out on manganese borides.

Support from JST Mirai Program (JPMJMI19A1) is acknowledged.

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Boron-based main group catalyst for non-oxidative methane coupling

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Nonoxidative coupling of methane represents a long-standing challenge in heterogeneous catalysis, as it requires activation of the carbon–hydrogen (C–H) bond, controlled carbon–carbon (C–C) bond formation, and effective hydrogen management without relying on oxidants. We discovered a low-temperature C–H activation and nonoxidative C–C coupling of methane with another methane, and also with CO_2, over atomically dispersed titanium–aluminum–boron nanopowder. Methane activation is initiated at 800 K, approximately 700 K below the gas-phase decomposition threshold, leading predominantly to ethylene formation. Coupling with CO_2 produces acetic acid. The active site of the catalyst is a tandem site of a single Ti atom surrounded by boron. The Ti-B motif enables methane adsorption and C–H activation, and the boron network acts as a reversible hydrogen reservoir. The same motif successfully activates CO_2. The metalloid nature of boron enables versatile bond activation, rendering the catalytic system comparable to platinum group metals.

h-BN large wafers - growth, properties, and applications

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Hexagonal boron nitride (h-BN) is an emerging ultrawide bandgap (UWBG) semiconductor that holds immense promise for revolutionizing electronic and photonic devices. Within the III-nitride family, h-BN remains relatively underdeveloped compared to its counterparts; however, it boasts remarkable characteristics, including a 6 eV bandgap, a high breakdown field of 12 MV/cm, and an impressive in-plane thermal conductivity of 550 W/m·K. Furthermore, h-BN serves as a host for optically stable single-photon emitters and qubits, and its 2D form is an ideal template and insulating barrier for graphene-based heterostructures. Beyond photonics, h-BN is uniquely suited for direct-conversion solid-state neutron detectors due to the exceptional thermal neutron cross-section of B-10 (3840 barns).

In this presentation, we provide an overview of our group's recent achievement in synthesizing large-diameter (up to 6-inch) h-BN quasi-bulk crystals (epitaxial layers hundreds of microns thick) using hydride vapor phase epitaxy (HVPE) [1-4]. We discuss the fundamental optical and electrical properties of these crystals, alongside their performance as hosts for single-photon emitters and quantum qubits. Benchmarking against state-of-the-art mm-sized bulk crystals reveals a well-defined stacking sequence and long-range order along the c-axis. We have demonstrated a record-high thermal neutron detection efficiency of 60% [1-3] and a practical efficiency of 5% for 14.1 MeV (D-T) fusion neutrons [4]. These developments represent a critical milestone in advancing h-BN crystal growth toward electronic-grade quality for high efficiency neutron detectors, power electronics, quantum information technology, and beyond.

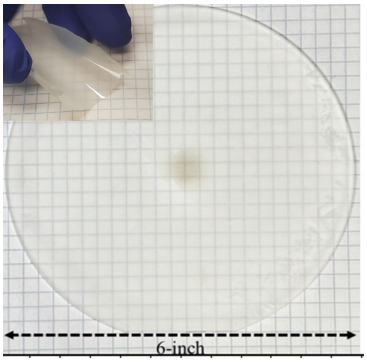

Figure 1. (a) Optical image of a freestanding h-BN wafer of 6-inches in diameter produced by HVPE. The inset shows that these freestanding h-BN wafers are flexible [after Ref. 2].

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Towards a Broad-Spectrum Catalyst for Aliphatic Polymer Breakdown

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This talk will describe some of our efforts to generate well-defined organometallics on oxide surfaces that behave similarly to weakly coordinating anions.[1] The ion-pairs formed on oxides of this type are generally applied as catalysts in olefin polymerization reactions,[2] one of the largest industrial applications of surface organometallic chemistry. The chemical understanding of how catalytically active ion-pairs form and/or self-assemble has led us to apply these finding to generate organometallic sites that break down polyolefin plastics. For example, we showed that sulfated aluminum oxide (**SAO**) reacts with $Ta(=CH^tBu)(CH_2{}^tBu)_3$ to form organotantalum species that react with H_2 to form electrophilic tantalum hydride sites that breakdown high-density polyethylene (HDPE) or isotactic polypropylene (iPP) to aliphatic products in the presence of H_2.[3] Our most recent results represent a pivot to that considers some of the more general challenges in processing plastic waste on the massive scales that would be needed to remedy this challenge. In particular we are leveraging our understanding of reactive sites on surfaces to activate C–H bonds in polymers to "crack" these rather inert materials into oils that can be processed further. Two stories describing the reactivity of pyrosulfate sites on zirconium oxide, which form extremely strong Lewis acid sites,[4] and a fluoriniated amorphous silica alumins (F-ASA) will be described.[5] The latter material is among the most active catalysts for aliphatic polymer breakdown currently known. Structural features that make this catalyst unique will be discussed.

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Theoretical Characterization of Small Boron Clusters Based on the Semiclassical B–B Potential

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An updated semiclassical approach[1,2] to calculating the electronic structure for bounded systems of atomic allows, in principle, the construction of paired interatomic potentials in analytical form. Implementation of such a program for boron atoms yielded[3,4] a semiclassical B–B interaction potential in a form integrable into elementary functions. An analytical representation of its dependence on the interatomic distance proved useful for estimating[5] ground-state parameters (specific binding energy, bonds length, zero-point vibrations frequency, static atomic charges, dipole moment, etc.) for all-boron small clusters, which prefer (quasi)planar structures and are considered as building blocks for growing two-dimensional boron-based materials[6] promising in many modern advanced technologies. Here, the electronic structure of small boron clusters will be theoretically characterized based on the semiclassical B–B potential.

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Accelerating the Discovery of Superhard Borides for Extreme Environments

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Superhard materials (Vickers hardness > 40 GPa) are critical for applications in manufacturing, cutting technologies, and energy systems, where both mechanical robustness and thermal stability are required. Among candidate systems, transition metal borides and boron-rich compounds have emerged as particularly promising; however, the discovery of new boride-based superhard materials has largely relied on empirical design principles derived from a narrow chemical space. This talk introduces machine learning as an alternative approach to overcome these limitations. The work highlights the power of combining experimental mechanical property data with constructing an ensemble machine learning model trained to predict load-dependent hardness, thereby directly moving beyond heuristic strategies. The model's predictive performance was validated by testing a range of compounds, including a complex, large, and disordered metal borosilicide, demonstrating its utility for even the most complex systems. The talk further addresses a key real-world challenge by outlining strategies for predicting hardness at elevated temperatures and estimating the onset oxidation temperature, both essential for developing materials that can withstand extreme industrial conditions. Together, these strategies demonstrate how machine learning can accelerate the discovery of superhard, thermally stable materials, enabling a data-driven approach to designing compounds for extreme environments.

Computational search for stable magnetic and superconducting systems

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I will discuss the status of computational electronic-structure-based searches for new stable magnetic and superconducting systems, with a focus on borides. The current successes and failures of artificial intelligence, machine learning, and high-throughput methods for theoretical predictions of solid-state magnetic materials will be discussed across different system types. More details will be provided for high-throughput screening of novel magnetic materials and their properties. Specific property-dependent peculiarities of such screenings will be demonstrated for magnetic structure determination, the critical temperature of the magnetic phase transition, magnetic anisotropy in rare-earth magnets, altermagnetism and electron-phonon superconductivity. Complications of 'true' theoretical predictions of realistic systems will be shown. Numerous examples of experimentally verified predictions for stable systems with different magnetic orders will be shown, and possible applications will be discussed.

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Self-compensation and Bonding Conversion in Semiconducting Quasicrystalline Approximants, Related Crystals and Amorphous

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Self-compensation mechanisms against carrier doping and bonding conversion induced by transition-metal addition are investigated in semiconducting quasicrystalline approximants, related boron crystals, and amorphous semiconductors.

The α- and β-rhombohedral phases of pure boron are considered to be 0/1–2/0 rhombohedral approximants of icosahedral quasicrystals [1]. In β-rhombohedral boron, although the ideal structure has holes in the valence band and is expected to be metallic, interstitial atoms and vacancies are spontaneously introduced to compensate the carrier imbalance, resulting in a semiconducting state. Even under electron doping with Li or Mg, structural rearrangements occur, maintaining charge neutrality and preventing metallization [2]. Similar self-compensation behavior is also observed in α-tetragonal boron [3] and boron carbide [4], where structural modifications effectively cancel the introduced carriers.

In contrast, amorphous semiconductors such as chalcogenide glasses and amorphous Si exhibit different self-compensation mechanisms. In chalcogenides, flexible coordination environments suppress effective carrier doping, while in amorphous Si, a high density of dangling bonds forms localized states that trap carriers.

On the other hand, bonding conversion induced by transition-metal addition shows a clear contrast between boron-based materials and amorphous Si. In β-rhombohedral and amorphous boron, a small amount of transition-metal atoms converts covalent bonding into metallic bonding, leading to a semiconductor-to-metal transition [5]. This behavior originates from the common B_{12} cluster units [6]. In amorphous Si, however, much higher metal concentrations are required to induce such a transition.

These results highlight that self-compensation and bonding conversion strongly depend on the local structural units and bonding nature, with boron-based systems exhibiting unique characteristics associated with cluster structures.

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Photo irradiation effects on frustrated boron

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β-rhombohedral boron (β-boron) is known to have extremely complex crystal structure based on icosahedral structural motifs, wherein, the building units, B_{12} and B_{28}, exhibit contrasting ionization tendencies: icosahedra as anionic (B_{12}^{-2}) and fused-icosahedra as cationic ($2(B_{28})B^{+3}$). The framework of β-boron, sometime labeled as rh105, which can be described as $4B_{12} + 2(B_{28})B$, lacks 5 electrons (4 x [-2] + 3 = -5) to form a conventional semiconducting band structure: fully occupied valance band and completely empty conduction band. Very interestingly, β-boron approximately achieves such a semiconducting band structure by introducing interstitials and vacancies in a way that the network of point defects that can be mapped on an "anti-ferromagnetic Ising model on an expanded kagome lattice", whose ground state is degenerate and disordered.

It has been being pointed out that these defects may be mobile and can diffuse easily via thermal activation and/or photo illumination, albeit existing evidenes are indirect: change in optical absorption profile at certain temperatures, kinks in tenperature dependence of electrical conductivity, persistant photo conductivity.

Another interesting property of β-boron, which may be related to the presence of macroscopic amount of intrinsic defects due to imperfect filling of valence band, is high propensity of impurity inclusion during synthesis and/or thermal treatment of β-boron. Such tendency was stated in the report on the discovery of β-boron.

In this presentation, we will first overview the properties of β-boron relevant for recently discovered photo-induced phase transition of β-boron that may be driven by hydrogen intake and discharge. We will then shed light on mechanisms of photo-induced process in boron that could be used for applications such as switch and memories.

Part of this work was performed under the auspices of the U.S. DOE by LLNL under contract DE-AC52-07NA27344 and supported by the Computational Materials Science Program of the U.S. DOE, Office of Science Basic Energy Science Program.

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Harnessing boron chemistry in molten salts: synthesis, reactivity, and properties of original nano-objects

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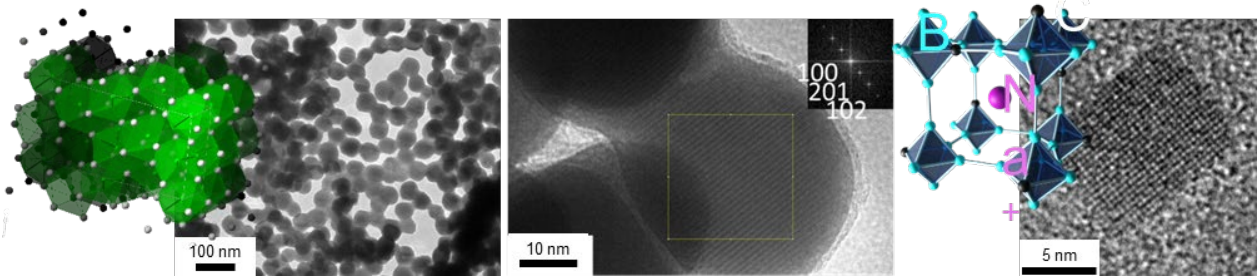
The various properties of boron-based inorganic solids[1–3] include superconductivity,[1] hardness,[2] thermoelectricity,[4] luminescence, and (electro)catalysis.[5] In nano-objects, these properties are deeply impacted: increased hardness, tunable luminescence, and enhanced (electro)catalytic activity have been demonstrated.[5] Therefore, exploring boron compounds at the nanoscale enables the emergence of original materials.[1,3,6] The strong covalent character of these solids however imposes harsh synthesis conditions accompanied by large crystal growth. Hence, synthesizing boron-based nano-objects remains a key challenge in the exploration of these materials. We will focus on the use of inorganic molten salts to overcome the challenge of boron-based nanomaterials synthesis.[1,3] Performing chemical reactions in inorganic molten salts is a way to trigger liquid-phase reactivity at temperatures that usually pertain to solid-state reactions. This conditions enable the production of strongly covalent boron-based compounds, especially borides and boron carbides. We will discuss the conversion of metal nanoparticles into size-controlled boride nanocrystals, the incorporation of additional p-block elements,[5] the production of 2D borides (MBenes) and the synthesis of boron carbide nanocrystals. We will show how synchrotron radiation, especially *in situ* X-ray diffraction and scattering, unveils complex crystallization pathways during the synthesis and highlights key synthesis parameters.[5] The promising performances of these nanomaterials for electrocatalytic water splitting[8] and for the development of superhard materials wil also be discussed.



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Recent Progress of Hydrogen Boride Nanosheets

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Hydrogen boride (HB, borophane, or hydrogenated borophene) nanosheets which are composed of boron and hydrogen at a 1:1 ratio can be formed by an ion-exchange reaction between protons and magnesium cations in magnesium diboride with exfoliation [1,2]. In the HB nanosheets, boron atoms form a hexagonal 2D network, in which hydrogen atoms are bound to boron by 3-center-2-electron bonds (B–H–B) and 2-center-2-electron bonds (B–H) [3,4]. Experimental studies have clarified that HB nanosheets exhibit solid acid catalytic activity [5,6], metal ion reducibility [7], gas-sensor applicability [8], stability against water [9, 10], CO adsorption/ conversion property including C-C coupling [11], a light-responsive hydrogen release function [12-15], electric field induced hydrogen release function [16] and material for inactivate viruses, bacteria, and fungi within minutes in the dark conditions [17]. In the presentation, recent progress of HB nanosheets including hydrogen release mechanism [4,18-20] will be introduced.

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(B,C) and (B,C,Si) at high pressure: modelling and synthesis at high temperature

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Boron cabide ceramics have exceptional mechanical properties, like e.g. the ceramics' highest Hugoniot Elastic Limit (HEL) around 17-20 GPa. Yet under a dynamical load above 20 GPa, they gradually lose their mechanical strength. While the occurrence of a phase transition around 20 GPa has been excluded so far, the formation of amorphous shear bands, as well as the formation of boron vacancies in the C-B-C chains of boron carbide, have been observed when entering the plastic deformation regime [1]. Our aim is to reinforce the chains, following several paths: by directly forming the carbon-carbon bonds that is predicted by theory to formed subsequently to the occurrence of chain vacancies; By inserting silicon into the chains. In the presentation, we discuss both routes, the first one by reporting principally density functional theory (DFT) calculations the formation of C-C chains in alpha-boron and boron carbide [2,3], the second one by reporting DFT calculations, thermochemistry CALPHAD calculations [4], and high pressure syntheses.

Calculations have been performed with the Quantum ESPRESSO software. Access to high performance computing (HPC) resources have been granted by the IDRIS, CINES, TGCC national centers (GENCI Project 2210 and TGCC special allocation) and by the 3Lab cluster of Ecole Polytechnique. We acknowledge support from the ANR through the BCSi project.

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Lanthanide Borocarbides with Hydride Interstitials

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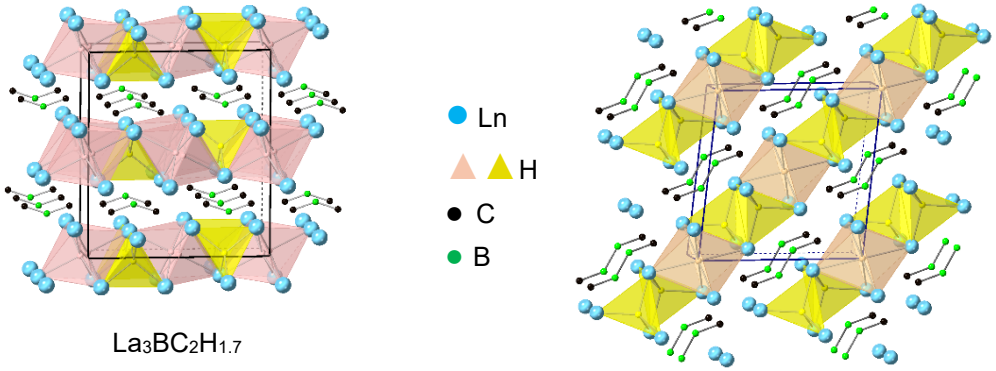
Eutectic mixtures of an early lanthanide metal with a late first row transition metal (Ln/T) can be used as fluxes for the growth of lanthanide-rich intermetallic compounds. Hydrocarbons such as anthracene react in these fluxes, acting as a source of carbon and hydrogen. When boron is included as a reactant, lanthanide borocarbides are formed as large crystals, with hydrogen occupying tetrahedral and octahedral interstitial sites. $Ln_3BC_2H_x$ compounds with the $Ca_3C_3Cl_2$ structure type form with Ln = La-Pr; the structure features 3-atom borocarbide chains. The $La_3BC_2H_{1.7}$ analog is superconducting below 5 K.[1] Increasing the amount of boron reactant leads to formation of $Ln_4B_2C_2H_x$ (Ln = La or Ce) with the stuffed Nd_2BC structure type, which features 4-atom borocarbide chains.[2] The lanthanide analog is superconducting below 4 K, and the cerium analog exhibits antiferromagnetic ordering at 7 K. The hydride interstitials in these compounds can be substituted by fluorides by using decafluorobiphenyl as a reactant.[1,3] The possible filamentary nature of the superconductivity in these materials will be discussed.



$La_3BC_2H_{1.7}$ $Ce_4B_2C_2H_{2.4}$

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Direct observation of an fcc-type ordered phase in CrCoNi-based alloy formed via a boron-stabilized amorphous phase by TEM/STEM

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The face-centered cubic (fcc)-type ordered phases ($L1_2$,- and/or $D0_{22}$-types) were developed in the $(CrCoNi)_{80}Si_{10}B_5P_5$ alloy by annealing a precursor amorphous phase which synthesized by the rapid quenching. To obtain the CrCoNi-based amorphous alloy as a precursor for chemical ordering through annealing, boron (a well-known glass-forming element) and Si and P were added to the CrCoNi mother alloy. Anomalous X-ray scattering analysis has already confirmed that the annealed $(CrCoNi)_{80}Si_{10}B_5P_5$ sample exhibits superlattice reflections from an $L1_0$-, $L1_2$-, and/or $D0_{22}$-type ordered structure [1]. The 4D-STEM dataset, obtained using nano-beam electron diffraction, indicates that the fcc(the main phase) and several crystalline phases coexist with fcc-type chemically ordered phases in the annealed sample of the liquid-quenched alloy. Superlattice reflections corresponding to the 001 and 110 reciprocal positions appear in the two-dimensional nano-beam electron diffraction pattern of the 4D-STEM dataset. From a microstructural investigation based on TEM/STEM observations, the grain size and shape of the ordered phase were approximately 20 nm and irregularly shaped, respectively. The ordered phase grains apparently have a higher concentration of Cr and B than the mother alloy composition, as revealed by simultaneous STEM-spectroscopy. It was possible that the ordered phase is a cubic anti-perovskite-type $(Co, Ni)Cr_3B_x$ compound.

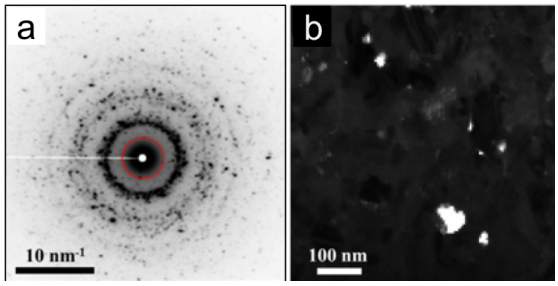

Figure 1(a) Integrated electron diffraction pattern from 4D-STEM data cube of the annealed $(CrCoNi)_{80}Si_{10}B_5P_5$ alloy. (b) Reconstructed pseudo DF-STEM image using the intensity of the diffraction pattern selected with the red circle shown in (a). The red circle corresponded to the position of the wave vector of the fcc-type ordered phase.

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Borides of manganese with platinum group metals

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Despite manganese is cheap, abundant and in its compounds generally introduces interesting magnetic behaviour, information on ternary combinations with platinum metals and boron are still scarce. The present talk will provide an overview on the current state on ternary phase relations, compound formation, crystal structures and physical properties in the systems Mn-{Ru,Os,Rh,Ir,Pd,Pt}-B. Results are based on micrografic studies (EPMA, EDX, WDX), X-ray single crystal and powder diffraction, SAED-TEM analyses and physical property studies (specific heat, electric conductivity, magnetism, hardness) in selected cases also backed by DFT calculations.

Mechanical Activation-Assisted Synthesis of Transition Metal Borocarbide and Boronitride Nanocompounds for Electrochemical Energy Storage

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Transition metal borides, carbides, and nitrides have recently attracted significant attention as emerging electrode materials for advanced energy storage systems due to their exceptional electrical conductivity, chemical stability, and multifunctional properties [1-2]. In this study, the synergistic interaction between transition metals (e.g., Mo, Fe) and boron combined with carbon or nitrogen is systematically investigated through a mechanical activation-assisted synthesis strategy. By employing melamine ($C_3H_6N_6$) as both carbon and nitrogen precursors, the effects of precursor stoichiometry on phase evolution, structural stability, and electrochemical behavior were comprehensively examined. The proposed synthesis route enabled the formation of novel Mo_xBC- and $Fe_x(BN)_2$-based nanophases, as representative examples of transition metal borocarbides (TMBCs) and transition metal boronitrides (TMBNs), respectively. First-principles phonon band dispersion calculations confirmed the dynamical stability of the ternary structures, while electronic structure analyses revealed their metallic character. Furthermore, the close agreement between simulated and experimental X-ray diffraction (XRD) patterns together with Raman spectra provided strong evidence for the experimental realization of these ternary phases and confirmed the consistency between theoretical predictions and experimental findings regarding their structural and vibrational characteristics. The electrochemical performances of the synthesized nanocompounds were evaluated as supercapacitor electrode materials. The samples exhibiting the highest phase purity and finest particle sizes (< 80 nm) demonstrated enhanced electrochemical performance, delivering high specific capacitance and energy density values. In addition, the electrodes exhibited remarkable power densities in the range of 40–70 kW kg^{-1}, indicating excellent rapid charge–discharge capability. All assembled devices also showed outstanding long-term stability, maintaining Coulombic efficiencies above 98 % after 10000 cycles. These findings highlight the strong potential of novel TMBCs and TMBNs nanocompounds as scalable and high-performance multifunctional material platforms for next-generation electrochemical energy storage technologies.

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Transforming Layered Metal Borides through Dissolution–Recrystallization: Scalable Routes to Functional Boron Nanomaterials

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Nanosheets derived from layered metal borides are emerging as an important class of boron-rich 2D materials with significant promise for electrochemical, electronic, and catalytic applications. In this talk, I will discuss our discovery of dissolution–recrystallization mediated transformation pathways in layered diborides and their role in enabling synthesis of low-dimensional boron-based nanostructures.

We showed that MgB_2 and related layered borides can undergo n dissoear completelution under mild chemical conditions, followed by recrystallization into nanosheets, nanoflakes, and nanodots through nonclassical growth pathways involving prenucleation clusters and oriented attachment. These processes generate colloidal dispersions of chemically active boron-rich nanostructures with micron scale lateral dimensions and nanoscale thickness.

The presentation will further highlight the utilization of these nanosheets in lithium-ion storage, dielectric systems, and polymer nanocomposites where their unique interfacial chemistry and structural features contribute to enhanced functional behavior.

Collectively, these studies establish dissolution–recrystallization as a versatile synthetic framework for transforming layered borides into functional low-dimensional materials and provide new insights into the dynamic chemical behavior of metal borides in reactive environments.

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Layered MAX and MAB Phases: Synthesis-Driven Pathways to Functional Ceramics

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The discovery and synthesis of new inorganic layered materials remain central to advances in energy, extreme-environment technologies, and functional materials design. Among these, MAX phases — layered ternary carbides, nitrides, and carbonitrides — have attracted considerable attention because they uniquely combine ceramic and metallic characteristics, including high-temperature stability, damage tolerance, electrical conductivity, and machinability. Their exceptional chemical flexibility also makes them an ideal platform for exploring composition–structure–property relationships.

In this talk, I will present our recent efforts toward the synthesis of novel MAX phases, including previously unexplored carbonitrides, compounds incorporating unconventional A-site elements, morphology-engineered composite architectures and their 2D derivatives (MXenes). Particular emphasis will be placed on how compositional tuning and structural design influence phase stability and functional behavior relevant to high-temperature applications.

I will also discuss emerging work on structurally related layered borides (MAB phases), a rapidly growing class of boron-containing materials that exhibit intriguing magnetic and electronic properties. These studies highlight the broader opportunities enabled by chemically complex layered borides and related compounds for discovering new functionalities and expanding the design space of advanced materials.

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Title: Elelctron Diffraction for Natural Product Discovery and New reactions of vinyl carbocations.

Abstract: In this talk I will discuss our recent efforts to utilize phenyl and vinyl carbocations in C–H functionalization reactions. We will describe how these high-energy dicoordinated carbocations can be generated under mild conditions and utilized in the selective C–C bond forming reactions of simple hydrocarbons. Moreover, we will discuss our efforts to understand the mechanism of these reactions through computational chemistry, kinetics, electron microscopy, and isotopic labeling studies. We will also present recernt efforts to apply electron microscopy to problems in organic chemistry (specifically natural product discovery) through the use of MicroED and other CryoEM modalities.

Biography: Prof. Nelson earned a B.S. in Chemistry from University of California at Berkeley in 2005, after transferring from City College of San Francisco. He earned a Ph.D. from the California Institute of Technology in 2013, where he studied natural product synthesis with Brian Stoltz. After postdoctoral training at University of California at Berkeley in asymmetric catalysis with Dean Toste, Prof. Nelson joined the UCLA faculty in 2015. In 2021 he joined Caltech's Division of Chemistry and Chemical Engineering. Prof. Nelson's research program is focused on the development of enabling technologies for chemical synthesis. His group focuses on this goal through two primary avenues of research. 1) In their structural chemistry subgroup they develop new electron microscopy techniques that enable the characterization of complex molecules, often unattainable using traditional methods. 2) Their synthetic subgroup focuses on the development of new chemical reactions that will enable the efficient and rapid synthesis of bioactive compounds.

Ternary compounds of boron with transition metals under OER conditions

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Water electrolysis is a key process for producing hydrogen - a clean and sustainable energy carrier. However, wide application of this electrochemical technology onto the industrial scale still lacks of the long-lasting and more efficient electrocatalysts for the kinetically sluggish oxygen evolution reaction (OER). Refractory boron materials with transition metals get more and more into focus of research.

The OER performance of intermetallic precursors in the bulk state allows avoiding the detrimental effects of binders and/or supports and assessing the intrinsic activity and stability of electrode material. The (electro)chemical behavior of intermetallic compounds Mo_2TMB_2 (*TM* = Fe, Co, Ni) under OER conditions has been investigated using electrochemical data combined with extensive bulk- and surface-sensitive material characterization. *In situ* formation of *TM*-rich amorphous layers, composed of their oxides and hydroxides, accompanied with partial dissolution of molybdenum and boron was observed for all three compounds. The degree of molybdenum and boron dissolution depends also on the nature of *TM* oxides/hydroxides formed on the surface of Mo_2TMB_2. While the *in situ*-formed Fe_2O_3 and $Ni(OH)_2$ on the surface are the origin of OER inactivity, the simultaneous presence of Co_3O_4 and $Co(OH)_2$ on the surface of OER-exposed Mo_2CoB_2 electrode allows OER start at lower overpotential (ca. 270 mV) compared to elemental Co.

Significantly lower OER overpotentials for $TMCo_3B_2$ materials (ca. 270 mV) compared to elemental Co (ca. 320 mV), almost doubled current density values at maximum potential reaching up to 0.7 A cm^{-2} for $ZrCo_3B_2$ and up to 1.1 A cm^{-2} for $HfCo_3B_2$ as well stability of their OER activity for almost 500 h reaction period bring forward those intermetallic compounds among other known electrocatalysts. The highly OER active and stable $ZrCo_3B_2$ and $HfCo_3B_2$ electrodes illustrate the importance of crystal structure and chemical bonding of intermetallic compounds, remarkably influencing the OER performance.

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Transition-Metal Boron Monofluoride Complexes

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In 2019, our group reported the isolation and full characterization of the terminal boron monofluoride $Fe(BF)(CO)_2(CNAr^{Tripp2})_2$ (Ar^{Tripp2} = 2,6-(2,4,6-(*i*-Pr)$_3C_6H_2)_2C_6H_3$). When bound to this mixed isocyanide/carbonyl FeL_4 fragment, the BF ligand proved to be both a strong σ-donor and highly efficient π-acceptor, which is in line with the predicted properties of boron monofluoride. In this presentation, additional aspects of the nature and chemistry available to the BF ligand are discussed. Consistent with its strong π-acceptor character, the BF ligand is a site of high electrophilicity within $Fe(BF)(CO)_2(CNAr^{Tripp2})_2$. As shown through reactivity studies, Lewis bases can readily bind to the BF unit, with or without displacement of the fluoride substituent. These findings have enabled the transformation of BF into other metal-coordinated diatomic molecules. Also addressed is the synthesis of other transition-metal BF complexes.

Phonon Transport and Impurity Effects in Ultrahigh-Thermal-Conductivity Cubic Boron Arsenide

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Cubic boron arsenide (BAs) has emerged as an ultrahigh-thermal-conductivity semiconductor for advanced thermal management. High-quality BAs single crystals exhibit room-temperature thermal conductivity exceeding 1000 W m^{-1} K^{-1}. This unusual behavior arises from favorable phonon band features that suppress three-phonon scattering, while higher-order four-phonon scattering plays an important role in limiting the intrinsic thermal conductivity. In this talk, I will discuss the effects of impurities on thermal and electrical transport in BAs. Trace impurities, such as Si, C, O, H, Te, and I, were detected by time-of-flight secondary ion mass spectrometry and electron probe microanalysis measurements. Some of these impurities can introduce p-type carriers and reduce carrier mobility. Furthermore, these impurities can enhance phonon scattering, leading to large variations in thermal conductivity among as-grown crystals. In addition, thermal expansion and Grüneisen-parameter measurements provide insight into lattice anharmonicity and indicate that BAs has a better thermal-expansion match with common semiconductors than diamond and cubic boron nitride. These results highlight both the promise of BAs for thermal management and the importance of impurity and defect control in realizing its full potential.

Unlocking Charge Transport at Polar c-BN/Diamond Heterointerfaces: A Path to n-Type Diamond Electronics

Dr. Mahesh R. Neupane

ARO/ARL

Heterointerfaces combining cubic boron nitride (c-BN) and diamond present a compelling architecture for next-generation ultra-wide bandgap (UWBG) electronics that leverages their identical crystal structures, exceptional thermal stability, and minimal lattice mismatch (1.4%). While diamond possesses outstanding physical properties, its development is severely bottlenecked by the lack of shallow, efficient n-type dopants. This work demonstrates that n-type c-BN can serve as an effective surface transfer doping layer to overcome diamond's doping limitations, enabling viable n-type diamond-based field-effect transistors and seamless integration with III–V semiconductor technologies.

Due to the polar nature of the (100) interface, these heterojunctions offer exceptional tunability. Using first-principles calculations, we show that precise interfacial stoichiometry control can induce either n- or p-type conductivity—generating high-density, 2D electron or hole gases (2DEG/2DHG)—and shift band offsets by up to 2 eV between Type-I and Type-II alignments. This theoretical framework is directly corroborated by recent experimental synthesis, which confirms that stoichiometry manipulation dictates both structural stability and electronic behavior. Ultimately, these findings clarify the underlying physics of polar c-BN/diamond interfaces, establishing a concrete design paradigm for high-performance UWBG device structures.

Acknowledgment: This work was conducted under the Advanced Power Electronic and Extreme-Radio Frequency (APEX) project under the Applied Research for the Advancement of Science and Technology Priorities (ARAP) Program at DEVCOM ARL by Dr. Cody Milne under the supervision of Prof. Arunima Singh and Dr. Mahesh Neupane. This work was also supported by the Army Educational Outreach Program with DEVCOM ARL, and computational grants for this work were provided by the DoD High-Performance Computing Modernization Program at the U.S. Air Force Research Laboratory and Supercomputing Resource Centers.

Stability and Metallicity in Metastable Layered Metal Borides

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Layered metal borides possess a wide range of properties including strong chemisorption, catalysis, and energetic materials. The most interesting systems are those that are barely stable because they tend to contain transition metals in unusual configurations. In those systems, the boron serves as a scaffold whose strong metal-boron bonds bind the metals into an unfavorable coordination environment, which enables heavy metal adsorption, poison resistant catalysis, and potential rocket fuels. We will discuss the role of stability specifically in boron-based systems and show how the low stability enables exotic properties.

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Thermochemically-Driven Exchange Reactions for the Rapid Synthesis of Crystalline Metal Borides: Reaction Scope and Limitations, and their Investigation as Hydrogen Evolution Electrocatalysts

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Rapid reactions of two or more solids can be highly exothermic for thermochemically designed solid-state metathesis (SSM) reactions [1]. This presentation will highlight reactions of anhydrous metal halides intimately mixed with Mg and B powders that produce exothermic short-lived reactions where metal salts are reduced and crystalline metal borides grow in a transient molten $MgCl_2$ flux (~1400 °C). This rapid synthetic method produces single metal and solid-solution borides in the 3d MB (M=Fe, Co, Ni [2]) series and has been extended to several layered MB_2 early transition metal structures and 4d borides (*e.g.*, TiB_2, NbB_2, Pd_2B) and carbon black supported metal borides. Strategies for successful SSM reactions and thermochemical insights on the limitations for self-propagating SSM reactions will be presented. The metal borides and composite structures are examined as hydrogen evolution reaction (HER) electrocatalysts. Many of the crystalline SSM produced metal borides show good chemical robustness in acidic and basic electrocatalytic reduction experiments. Trends in HER activities will be described with respect to metal boride properties and boron content.

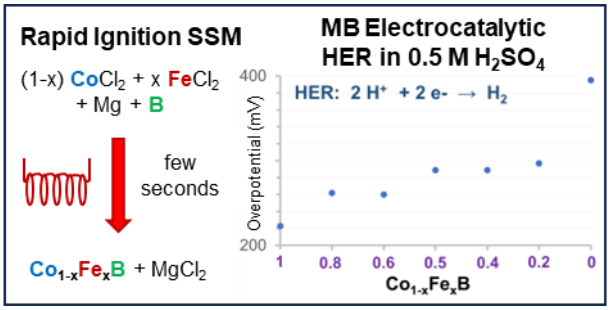

Figure. Rapid solid-solution SSM growth of $Co_{1-x}Fe_xB$ particles and their HER activity.

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Structural Characterization of Boron Nitride and Oxide Materials by Dynamic Nuclear Polarization and Ultrahigh Field 35 T Solid-State NMR Spectroscopy

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Boron nitride and boron oxide materials have applications in electronic devices, ceramics, separations/membranes and heterogeneous catalysts. This talk will describe how dynamic nuclear polarization (DNP) or ultrahigh field 35 T solid-state NMR spectroscopy can be used for the structural characterization of boron nitride and related materials. We will show how $^{1}H \rightarrow ^{11}B$, DNP-enhanced surface-selective $^{1}H \rightarrow ^{15}N$, and $^{1}H\{^{14}N\}$ NMR spectroscopy experiments, can be used to detect armchair and zigzag terminated edges on exfoliated boron nitride nanosheets.[1] Ultrahigh-field 35 T ^{11}B solid-state NMR spectroscopy is shown to provide order of magnitude improvements in ^{11}B NMR resolution and sensitivity.[2] We describe the use of 35 T ^{11}B solid-state NMR spectroscopy to obtain detailed of oxidized boron nitride which are heterogeneous catalysts for the oxidative dehydrogenation (ODH) of propane.[2,3] Notably at 35 T, ^{11}B double-quantum, single-quantum (DQ-SQ) homonuclear correlation spectroscopy can be used to obtain a detailed picture of boron connectivity and speciation.[2] Finally, we will also demonstrate that simple REDOR recoupling can be used to obtain 2D $^{11}B\{^{17}O\}$ dipolar HMQC NMR spectra and these techniques can be used to study the structure of highly active ODH catalysts consisting of boron oxide supported on activated carbon.[4,5]

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Boron-containing semiconductors and heterostructures are attractive for high-power, high-frequency, and extreme-environment electronics because of their wide bandgaps, strong bonds, and potentially exceptional thermal transport properties. However, their practical performance is often controlled less by ideal intrinsic properties than by synthesis-dependent crystal quality: point defects, extended defects, phase purity, bond disorder, and interfacial structure. In this talk, I will discuss how thermal conductivity and thermal boundary conductance can serve as sensitive, quantitative metrics for these forms of materials quality.

I will first describe recent advances from our group in ultrafast optical thermal metrology for high-thermal-conductivity thin films, including picosecond magneto-optic thermometry approaches that improve the ability to independently measure thin-film thermal conductivity and interface conductance in sub-micron films. I will then discuss two case studies where these measurements reveal materials quality in boron-containing systems. The first is BN/diamond heterostructures grown by plasma-enhanced chemical vapor deposition, where thermal transport distinguishes turbostratic and cubic BN phases, reveals depth-dependent disorder in nominally crystalline c-BN, and shows that sp^3-bonded c-BN/diamond interfaces conduct heat approximately three times more effectively than t-BN/diamond interfaces. The second is cubic boron arsenide, where measurements of high-purity single crystals reveal ultrahigh room-temperature thermal conductivity and an unexpectedly strong temperature dependence. In BAs, thermal conductivity provides a stringent benchmark for identifying the highest-quality crystals and a sensitive probe of how defects and phonon-scattering processes limit performance. Together, these studies show that thermal transport measurements provide a practical diagnostic of phase, bonding, disorder, interface quality, and crystal perfection across boron semiconductors and related materials.

Redox-Active Phosphines for Metal-Free Bond Activation

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Significant recent attention of the inorganic chemistry community has been focused on the metal-free redox bond activation. In our work on the development of catalytic systems, we utilize fundamental principles of chemical bonding to design and create a unique electronic environment for main-group element reactive centers.

We designed a metal-free boron cluster-containing molecular framework that possesses two important features normally reserved for transition metals: the presence of Lewis basic binding sites and the ability to reversibly cycle through two-electron redox states.[1] The synergy between these two properties resulted in transition-metal type reactivity in the metal-free main-group element system. The use of electron-rich phosphine groups attached to the electron-accepting carborane cluster allowed for the spatial separation of frontier orbitals of the molecule and ambiphilicity of carboranyl diphosphines.[2] We found that their reactions with main group hydrides, alcohols, and ammonia occur with phosphine groups acting as electrophiles.[3,4] We also demonstrated that the redox activity of the cluster can be coupled with the proton transfer from the phosphine groups.[5]

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SECTION 02

Oral Presentations

Conference section divider

From Solid State to Solution: High-Temperature Routes to B-functionalized Boron Clusters

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Synthetic modifications of icosahedral carborane molecules traditionally follow wet chemistry techniques utilizing solvent-based systems. In this presentation we showcase an alternative synthetic route; molten salt conditions that engender exopolyhedral functionalization that is not readily accessible via solvent based synthetic methods. Reported icosahedral carborane structures are dominated by carbon vertex substituted species due to the facile lithiation of carborane via organolithium reagents. The synthesis of boron vertex substituted variants of icosahedral carboranes has expanded in breadth in recent years, however there remain boron-element bonds that are not yet accessible by traditional solution-based synthesis. In my presentation, I will show how exopolyhedral B-Sn bonds can be forged by reacting B-mercurocarborane starting material in a $SnCl_2$ molten salt at temperatures exceeding 350 °C. Investigating the generality of this method, I replaced $SnCl_2$ with $GeBr_2$ as the molten salt medium resulting in an isolable carborane with an exopolyhedral B-Ge bond. Using disubstituted and trisubstituted B-mercurocarborane starting material with molten $GeBr_2$ generates products with two and three B-Ge bonds respectively. Moving from tetrel salts to triels, replacing $SnCl_2$ with InCl as the molten salt medium results in isolable carborane with an exopolyhedral B-In bond. This molten salt synthetic method provides the first opportunity to probe the electronic influence of B-bound carborane cages on these heavy main-group elements, demonstrating that the carborane substituents behave as strongly electron-donating groups, in contrast to conventional electron-withdrawing C-bound carborane substituents. Our findings also reveal an unusual thermal stability profile for several of the carborane-based molecules, challenging some of the longstanding assumptions in the field. I will further highlight the reactivity of these new main-group carborane systems and discuss how these building blocks can be leveraged for the construction of nanoscale architectures.

Collapse of the frustrated Shastry-Sutherland lattice in TmB_4 at high magnetic fields

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The two-dimensional Shastry-Sutherland (SSL) lattice belongs to important models in the field of quantum magnetism, it combines low-dimensionality, geometrical frustration and strong anisotropy. The metallic tetraboride TmB_4 with a tetragonal structure belongs to its best-known examples. In this contribution we present the development of its magnetization in magnetic fields B up to 60 T tilted from the easy magnetization axis c. Our results show that at temperatures below about 20 K considerable deviations from the easy-axis interpretation of magnetization, in which the magnetic moments of Tm-ions are oriented only parallel to c-axis, occur in magnetic fields above 30 T at deflection angles above 70 degrees. These critical values significantly influence the corresponding *magnetization* vs *temperature* phase diagram and point to a collapse of the SSL lattice in TmB_4. Moreover, the additionally observed high field anomalies suggest the existence of new quantum phases in this frustrated metallic tetraboride.

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Defect-Engineered β-B-derived nanosheets and Heterointerfaces for Efficient Electrochemical Water Splitting

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The development of boron-based two-dimensional materials has attracted increasing attention owing to their distinctive electronic structure and potential in electrocatalytic energy conversion. Despite extensive theoretical interest in borophene, the fabrication of stable, free-standing crystalline phases remains challenging. Here, we investigate an alternative route based on defect induced cleavage of β-rhombohedral boron to obtain ultrathin borophene-like nanoflakes. The proposed top-down methodology (ball-milling, modified Hummers method, ultrasound assisted liquid phase exfoliation) utilizes the presence of landscape of defects such as line and planar defects within the β-B framework to induce selective structural disintegration. This transformation results in the formation of β-B-derived nanosheets characterized by a high density of edge sites, amorphous regions, and partially oxidized surface domains. Such structural heterogeneity creates a large population of catalytically accessible centers capable of promoting both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). To further optimize charge-transfer kinetics and active-site utilization, the boron-derived nanoflakes were combined with transition-metal-containing phases, yielding hybrid heterostructures with improved interfacial electronic communication. Comprehensive structural, spectroscopic, and electrochemical analyses demonstrate that catalytic efficiency is governed by the interplay between defect concentration, surface reconstruction processes, and heterointerface formation. The results highlight defect-rich boron nanomaterials as a versatile platform for the rational design of next-generation bifunctional electrocatalysts for sustainable hydrogen production.

Thermal Dehydrogenation-Induced Magnesium Dispersion on Boron-Based Nanosheets

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Two-dimensional nanosheets can serve as platforms for dispersing metal species owing to their large surface area and accessible surfaces. Hydrogen boride (HB) nanosheets are particularly attractive boron-based 2D materials, offering both nanoscale boron frameworks and reactive hydrogen-related sites.[1] In this study, Mg-dispersed boron nanosheets were synthesized by heating HB nanosheets with ball-milled MgH_2 at 550 °C. Scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) analyses confirmed uniform Mg dispersion and suppression of Mg aggregation (Figure 1). Temperature-dependent X-ray diffraction patterns suggested that Mg diffused after H_2 release from HB and MgH_2, where it became trapped at hydrogen vacancies in the HB nanosheets. X-ray photoelectron spectroscopy and density functional theory results further indicated that the electronic states of Mg and B were similar to those in MgB_2, supporting the formation of Mg–B bonding. These findings demonstrate that HB nanosheets can act as a boron-based two-dimensional platform for stabilizing highly dispersed Mg species.

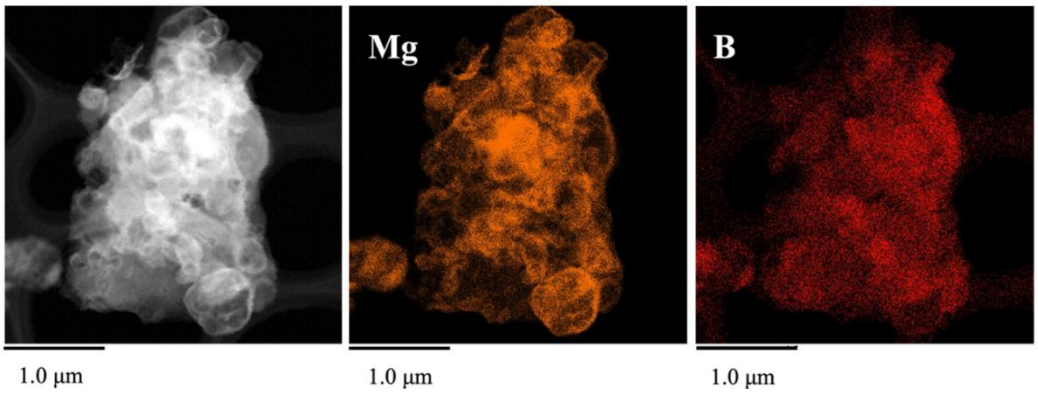

Figure 1. STEM and EDS mapping of highly dispersed Mg on boron nanosheets.

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Interlayer Hydrogen Spacing Regulates the Formation of Molecular Hydrogen in Hydrogen Boride Nanosheets

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Hydrogen carriers that enable efficient transport and on-demand release of H_2 are crucial for practical hydrogen-based energy systems. Hydrogen boride (HB) nanosheets, composed of boron and hydrogen in a 1:1 stoichiometric ratio, are promising safe and lightweight hydrogen carriers owing to their high gravimetric hydrogen density (8.5 wt %).[1] However, the mechanism of the multimodal H_2 desorption upon heating remains unclear. Here, we show that the interlayer H···H distances ($d_{H\cdots H}$) govern the multimodal desorption of H_2 especially in the lower-temperature range (Figure 1).[2] Infrared spectroscopy and temperature-programmed desorption (TPD) measurements revealed the occurrence of hydrogen depletion without changes in bonding configuration. The first to third nearest $d_{H\cdots H}$, along with the numbers of the corresponding H···H pairs, were systematically calculated for four possible interlayer stacking types. The calculated pair distribution closely matched the experimental desorption profile, indicating that lower-temperature multimodal H_2 desorption is governed by $d_{H\cdots H}$ distributions.

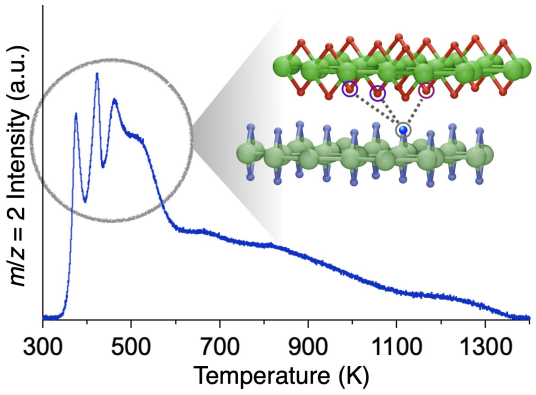

Figure 1. A representative multimodal H_2-TPD profile of HB nanosheets with a schematic illustration of interlayer H···H distances.

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Ternary Li-Ni-B compounds as promising catalysts for water splitting in alkaline media

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Intermetallic borides display a wide range of crystal structures, bonding motifs, and functional properties. Borides can be found as state-of-the-art materials in contexts such as permanent magnetism, superconductivity, magnetocaloric effect, and superhardness. [1–3] Most transition metal borides are metallic and are resistant to degradation in extremely acidic or alkaline environments.[3] This makes them ideal candidates for electrocatalysts for water splitting, which occurs as two half-reactions: oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). At present, the primary catalysts for both reactions contain critical platinum-group metals.[3,4]

While binary borides of first-row transition metals have been extensively explored for OER/HER activity, the class of ternary borides containing both an alkali metal and a first-row transition metal have not yet been studied. The relative scarcity of such phases may be due in part to the synthetic difficulties associated with obtaining them from direct reactions of the constituent elements.[5] In this work, we demonstrate the efficient synthesis of several phases in the Li-Ni-B ternary system using the hydride route, where the alkali metal is replaced by its salt-like hydride to enable better mixing and faster reactions.[6] We then show how post-synthetic ball milling to reduce particle size and increase the amount of exposed surface is crucial to realize the full electrocatalytic activity of these materials. The native Li-Ni-B compounds likely serve as pre-catalysts that generate an active layer of transition metal oxyhydroxides upon application of electric potential; the resulting surface states are investigated post-catalysis by XPS and TEM. The composition-structure relationship in the context of catalyst stability and activity for both alkaline OER and alkaline HER processes will be discussed for this family of Li-Ni-B compounds.

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Large Scale Production of Elemental Boron Powders via Metallothermic Reduction and Diborane Pyrolysis

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Elemental boron is a critical advanced material used in pyrotechnics, energetic systems, advanced ceramics, neutron shielding, semiconductors, and boride synthesis. Despite its technological importance, large-scale production of high-purity boron powders remains challenging due to boron's extreme oxygen sensitivity and purification difficulties associated with conventional reduction methods.

In this study, two industrial-scale elemental boron production routes are presented: magnesiothermic reduction of boron oxide and diborane pyrolysis. The first route involves self-propagating high-temperature synthesis (shs) using boron oxide and magnesium under inert atmosphere conditions, followed by crushing, milling, acid leaching, filtration, drying, and particle classification stages. This process enables the production of boron powders with purity levels exceeding 90–95 wt.% suitable for industrial applications.

In addition, the production of ultra-high-purity boron powder via thermal decomposition of diborane gas is discussed. In this process, diborane generated in situ is thermally decomposed at elevated temperatures under controlled inert atmosphere conditions, producing elemental boron powders with purity levels exceeding 99 wt.%. Particular attention was given to oxygen contamination control, gas handling safety, reactor atmosphere management, and post-processing conditions affecting powder oxidation and morphology.

The relationship between process parameters and powder characteristics such as purity, particle size distribution, and oxidation behavior was investigated under industrial manufacturing conditions. The presented results demonstrate that both metallothermic reduction and gas-phase pyrolysis routes provide scalable approaches for producing elemental boron powders tailored for different industrial requirements.

Keywords: elemental boron, diborane pyrolysis, magnesiothermic reduction, SHS, boron powder, large-scale production

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Synthesis of Sodium-Doped Hydrogen Boride toward Enhanced Hydrogen Adsorption Performance

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The realization of hydrogen society requires hydrogen (H_2) adsorbents that enable H_2 uptake and release under near-ambient conditions and exhibit high gravimetric H_2 density. Hydrogen Boride (HB) nanosheets are lightweight two-dimensional materials composed of positively charged hydrogen and negatively charged boron.[1] Previous theoretical studies predicted that the Na-doped HB monolayers exhibit the high H_2 adsorption property under near-ambient conditions. However, the synthesis of Na-doped HB and their H_2 adsorption property have not yet been demonstrated experimentally.[2] In this study, we developed a synthetic method to fabricate Na-doped HB via an ion-exchange method based on acid-base neutralization reaction.

Na-doped HB was prepared through the reaction between an acidic HB aqueous dispersion and a basic sodium hydroxide (NaOH) aqueous solution (Fig. 1). X-ray photoelectron spectroscopy (XPS) of the sample showed the Na 1s peak and the negatively charged B peak, indicating that Na was introduced by the substitution of H in HB. Fourier Transform Infrared Spectroscopy (FT-IR) spectra showed a change in peak shape near 1350 cm^{-1}, assigned to the in-plane B–H–B stretching vibration. Detailed peak separation analysis revealed the formation of compressed and stretched B–H–B groups, which is consistent with the theoretically predicted framework of Na-doped HB.[2] These structural characterizations demonstrate the successful synthesis of Na-doped HB. H_2 adsorption measurments showed that H_2 uptake was 0.092 wt% for HB and 0.17 wt% for Na-doped HB (298 K, 11.4 MPa), respectively. This indicates that Na doping in HB enhanced H_2 adsorption property.

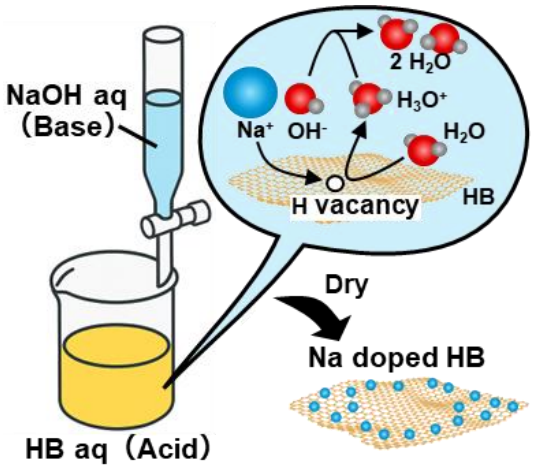

Fig.1 Synthesis Method of Na-doped HB

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Anisotropy-Driven Discovery of Rare-Earth-Free Permanent Magnets in Mn-Rich Mo_2FeB_2-Type Borides

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The discovery of rare-earth-free permanent magnets with high ordering temperatures is critical for next-generation energy and spintronic technologies. Here, we report the synthesis, magnetic characterization, and first-principles investigation of Mn-rich Mo_2FeB_2-type borides, $MoMn_2B_2$ and WMn_2B_2. Both compounds were synthesized as single phases by optimized solid-state reactions and crystallize in the tetragonal *P4/mbm* structure. Unlike their Mn-poor analogues, which exhibit spin-glass behavior, Mn enrichment stabilizes long-range ferromagnetic order with Curie temperatures of 420 K for $MoMn_2B_2$ and 390 K for WMn_2B_2. Magnetic measurements reveal that WMn_2B_2 exhibits hard-magnetic behavior with an intrinsic coercivity of 67.6 kA m^{-1} at 5 K, substantially exceeding that of $MoMn_2B_2$. Density functional theory identifies the ferromagnetic state as the magnetic ground state for both compounds and attributes the enhanced coercivity of WMn_2B_2 to its larger magnetocrystalline anisotropy (+0.27 meV per formula unit), arising from the stronger spin-orbit coupling of W. These results demonstrate that Mn enrichment suppresses magnetic frustration and promotes anisotropy-controlled ferromagnetism, establishing WMn_2B_2 as the first rare-earth-free permanent magnet in the Mo_2FeB_2 structural family and highlighting a promising strategy for designing multifunctional magnetic borides.

Densification of Transition Metal Diborides Produced by Pressureless Sintering

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Abstract

Using near net shaping methods such as isostatic pressing and slip casting coupled with pressureless sintering enables the production of complex geometries that are unobtainable through traditional hot-pressing. Slip casting is a traditional form of producing ceramic green bodies that utilizes a slurry to achieve fine detail and controlled geometry, while cold isostatic pressing utilizes pressure to achieve high green densities. This presentation will focus on the production of ultra-high temperature boride-based ceramics and challenges that can occur during processing. A variety of compositions have been studied including ZrB_2/HfB_2-based compositions and compositionally complex borides. Cast ceramics were produced as either hollow pieces, solid cast pieces, or layered composites and isostatic pressing was used to produce pellets for densification studies. Aspects of the processing including slip rheology, mold preparation, drying, and densification will be discussed. Densification was completed using pressureless sintering at temperatures ranging from 1800°C to 2300°C. Green densities were determined by using a non-contact 3-D optical profiler. Scanning electron microscopy was used to examine the microstructures of the resulting ceramics and energy dispersive spectroscopy was used to determine elemental distributions. Discussion will focus on challenges of the slip casting process and examples of compositions successfully produced by slip casting.

Acknowledgement

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Boron and Pnictogen Molecular Electronics

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Main-group molecular electronics is an emerging field that explores quantum transport through main-group backbones in molecular junctions.[1] To this point, most studies in main-group molecular electronics have focused on saturated oligosilane backbones, suggesting many new discoveries in molecular electronics will arise from interrogating quantum transport in a broader pallette of main group elements.[1] First, I will describe how the structure and bonding of 'B=N' and 'P=N' compounds manifest in single-molecule conductance studies. Next, I will discuss molecular conductance switches that operate by modulating the double-bond character in 'P=N' variants of the classic organic stilbene wire in response to exogenous chemical stimuli.[2] Efforts towards measuring air-sensitive, unsaturated main-group double bonds in a glovebox scanning tunneling microscopy break-junction system will be discussed. Together, these studies highlight how principles from main-group and organometallic molecular chemistry can be applied to exquisitely tune quantum electronic transport.

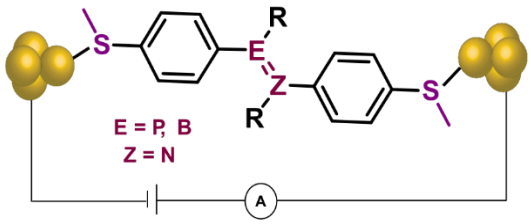

Figure 1. Boron and pnictogen molecular electronics

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B-H bond for hydrogen storage

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Hydrogen-rich systems composed of light elements such as B, C,and N have been extensively explored as hydrogen-storage materials. In this talk, I will first give a brief overview of borohydrides for hydrogen storage, such as room-temperature hydrogen cycling by $LiBH_4$, improved synthesis of $NaBH_4$. I will then discuss reactions between amine–borane complexes and amines that generate high-purity H_2 under ambient conditions. For example, the reaction between ethylenediamine bisborane (EDAB) and ethylenediamine (ED) yields unique B–C–N five-membered rings in the dehydrogenation product, in which one boron is tri-coordinated by three nitrogen atoms. I will also introduce BCN heteroicylic compounds such as 1,6;2,3-bis-BN cyclohexane—an isostere of cyclohexane with two adjacent BN pairs—which has an attractive hydrogen-storage capacity of >9.0 wt%, nearly twice that of 1,2;4,5-bis-BN cyclohexane.

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SECTION 03

Posters

Conference section divider

Anisotropy-Driven Discovery of Rare-Earth-Free Permanent Magnets in Mn-Rich Mo_2FeB_2-Type Borides

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The discovery of rare-earth-free permanent magnets with high ordering temperatures is critical for next-generation energy and spintronic technologies. Here, we report the synthesis, magnetic characterization, and first-principles investigation of Mn-rich Mo_2FeB_2-type borides, $MoMn_2B_2$ and WMn_2B_2. Both compounds were synthesized as single phases by optimized solid-state reactions and crystallize in the tetragonal *P4/mbm* structure. Unlike their Mn-poor analogues, which exhibit spin-glass behavior, Mn enrichment stabilizes long-range ferromagnetic order with Curie temperatures of 420 K for $MoMn_2B_2$ and 390 K for WMn_2B_2. Magnetic measurements reveal that WMn_2B_2 exhibits hard-magnetic behavior with an intrinsic coercivity of 67.6 kA m^{-1} at 5 K, substantially exceeding that of $MoMn_2B_2$. Density functional theory identifies the ferromagnetic state as the magnetic ground state for both compounds and attributes the enhanced coercivity of WMn_2B_2 to its larger magnetocrystalline anisotropy (+0.27 meV per formula unit), arising from the stronger spin-orbit coupling of W. These results demonstrate that Mn enrichment suppresses magnetic frustration and promotes anisotropy-controlled ferromagnetism, establishing WMn_2B_2 as the first rare-earth-free permanent magnet in the Mo_2FeB_2 structural family and highlighting a promising strategy for designing multifunctional magnetic borides.

From Solid State to Solution: High-Temperature Routes to B-functionalized Boron Clusters

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Synthetic modifications of icosahedral carborane molecules traditionally follow wet chemistry techniques utilizing solvent-based systems. In this presentation we showcase an alternative synthetic route; molten salt conditions that engender exopolyhedral functionalization that is not readily accessible via solvent based synthetic methods. Reported icosahedral carborane structures are dominated by carbon vertex substituted species due to the facile lithiation of carborane via organolithium reagents. The synthesis of boron vertex substituted variants of icosahedral carboranes has expanded in breadth in recent years, however there remain boron-element bonds that are not yet accessible by traditional solution-based synthesis. In my presentation, I will show how exopolyhedral B-Sn bonds can be forged by reacting B-mercurocarborane starting material in a $SnCl_2$ molten salt at temperatures exceeding 350 °C. Investigating the generality of this method, I replaced $SnCl_2$ with $GeBr_2$ as the molten salt medium resulting in an isolable carborane with an exopolyhedral B-Ge bond. Using disubstituted and trisubstituted B-mercurocarborane starting material with molten $GeBr_2$ generates products with two and three B-Ge bonds respectively. Moving from tetrel salts to triels, replacing $SnCl_2$ with InCl as the molten salt medium results in isolable carborane with an exopolyhedral B-In bond. This molten salt synthetic method provides the first opportunity to probe the electronic influence of B-bound carborane cages on these heavy main-group elements, demonstrating that the carborane substituents behave as strongly electron-donating groups, in contrast to conventional electron-withdrawing C-bound carborane substituents. Our findings also reveal an unusual thermal stability profile for several of the carborane-based molecules, challenging some of the longstanding assumptions in the field. I will further highlight the reactivity of these new main-group carborane systems and discuss how these building blocks can be leveraged for the construction of nanoscale architectures.

Mechanochemical functionalization and isomerization of oligosilane clusters.

Oluwakemi Dawodu, Jacob Seo, Ashley E. Pimentel, Elijah Mauga, Mario Imex Aguirre, Timothy A. Su

Saturated silicon clusters are part of an exciting new class of electron materials which exhibit unique quantum properties, such as destructive σ-quantum interference (σ-DQI). In bicyclo[2.2.2.]octasilane (Si222), this quantum property is associated with unprecedented insulation properties, however the functionalization of higher order oligosilane clusters has proven difficult due to limited solubility in a traditional solution phase approach. This presentation explores the use of ball milling mechanochemistry to functionalize and isomerize silicon clusters. The high energy transient forces applied during solution assisted grinding enable clean functionalization of these cluster dimers with electrophilic substituents, which allow the cluster to be wired between electrodes and probed for its molecular conductance. These reactions yield minimal byproducts and lead to desired difunctionalization over short time periods. Finally, I will discuss using ball milling mechanochemistry to convert various oligosilanes into their most thermodynamically stable isomer forms and their corresponding physical properties.

Ammonia-Induced Transformation of HB Nanosheets into BN-like Structures

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Hydrogen boride (HB) nanosheets are two-dimensional boron-based materials bridged and terminated by hydrogen atoms. In low-dimensional materials, heteroatom doping is an effective strategy for modifying functionality.[1] Previously, carbon doping into boron framework of HB has been investigated to tune their bonding structures.[2] In this study, we investigated ammonia-flow thermal processing of HB nanosheets as a route to induce nitrogen incorporation and structural transformation toward nitrogen-containing boron frameworks. HB nanosheets were thermally treated under continuous NH_3 gas flow at various annealing temperatures. The prepared samples, together with crystalline hexagonal boron nitride (h-BN) as a reference, were characterized by X-ray photoelectron spectroscopy (XPS), Fourier-transform infrared (FTIR) spectroscopy, and powder X-ray diffraction (PXRD).

As shown in Figure 1, XPS spectra revealed that the B 1s and N 1s peaks of the NH_3-treated samples annealed above 600 °C were similar to those of h-BN but appeared at lower binding energies by approximately 0.53 and 0.73 eV, respectively. These differences in binding energy may originate from low crystallinity and/or residual hydrogen-containing local structures in the HB-derived framework. FTIR spectra supported this interpretation, showing a gradual decrease in B–H vibrational modes and the emergence of B–N/B–N–B related bands with increasing annealing temperature. Both XPS and FTIR results indicate that the transformation was intermediate at 400 °C, where features of both HB and BN-like structures remained, whereas it was nearly completed at 600 °C, giving BN-like frameworks.

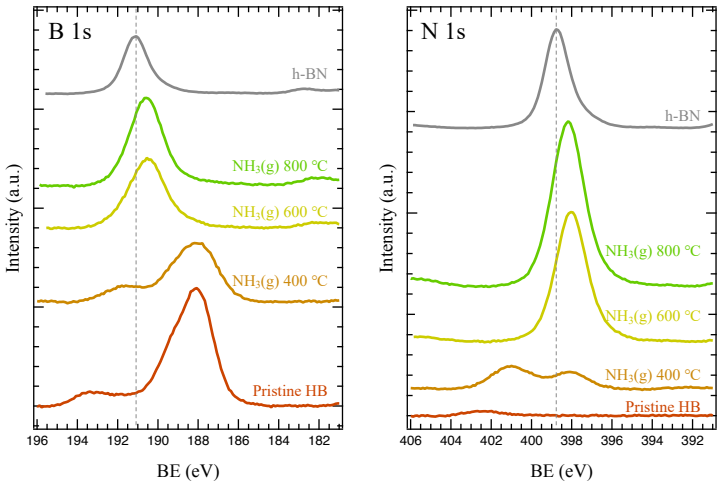

Figure 1. XPS spectra of B 1s and N 1s for pristine HB, NH_3-treated samples, and reference materials.

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Carborane Anions as Tunable Electrolytes for Mg and Li Batteries

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Carboranes have attracted considerable interest in battery research because their three-dimensional cage structures delocalize negative charge, giving rise to exceptionally weakly coordinating anions with outstanding chemical and electrochemical stability. These properties minimize ion pairing and promote efficient metal-ion transport, making carborane-based salts attractive electrolytes for magnesium- and lithium-based batteries. The development of practical Mg batteries has been hindered by the lack of electrolytes that combine high ionic conductivity, broad electrochemical stability, and compatibility with reactive metal anodes. In our laboratory, carborane-based magnesium and lithium salts are being designed and tuned to improve ionic conductivity, electrochemical stability, and long-term cycling performance. Magnesium electrolytes developed in our group have achieved ionic conductivities of up to 12.4 mS cm^{-1} and oxidative stability up to 4.2 V vs. Mg^{2+}/Mg.[1,2] This work highlights both foundational and recent advances in the development of carborane-based electrolytes for Mg and Li batteries, demonstrating the versatility of weakly coordinating carborane anions across multiple rechargeable battery chemistries.

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From Low-Temperature to Room-Temperature Rare-Earth-free Hard-Magnetic Borides of $Ti_3Co_5B_2$ -type

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$Hf_2FeOs_5B_2$, one of the first Os-rich quaternary variants of the prolific $Ti_3Co_5B_2$ structure type, was investigated computationally and experimentally. In its crystal structure, osmium builds a network of prisms, in which the other elements are located. The magnetic Fe atoms are found in face-connected Os_8 square prisms leading to Fe-chains with intra- and interchain distances of about 3.0 and 6.5 Å, respectively. Magnetic investigations show a metamagnetic behavior, whereby the antiferromagnetic interactions (T_N = 90 K) found at low magnetic fields change to ferromagnetic ones at higher fields. A hard-magnet hysteresis is found at 5 K with a 40 kA/m coercivity. In search for the first hard magnetic behavior at room temperature, we applied DFT calculations and identified $Hf_2FeOs_3Ir_2B_2$ phase combines high uniaxial anisotropy (E_{soc} = -5.45 meV/f.u.) and strongly positive exchange energy (E_{ex} = +21.80 meV/f.u.). Experiments validate the discovery of the first RT hard magnet of the $Ti_3Co_5B_2$ structure type with an intrinsic RT-coercivity of 36.6 kA/m and a Curie temperature of 490 K.

On Construction Secular Equation Determining Electronic Structure – Elementary Boron and Boron-Rich Materials

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A semiclassical method[1,2] of calculating the electronic structure of atoms and their systems leads to the construction of hydrogen-like atomic orbitals and, accordingly, integral representations of atomic and interatomic potentials in forms integrable into elementary functions. Based on the implementation[3,4] of such approach for boron, expressions will be derived for the matrix elements of the Hamiltonian and overlap integrals in the secular equation defining the electronic structure of all-boron and boron-rich materials, in particular, next-generation two-dimensional materials such as borophenes.

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Chemically Active Metal Diborides Based Nanosheets

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Metal diborides represent a set of ceramic materials consisting of layered boron honeycomb networks separated by metal atoms. These materials have gained substantial research interest owing to their exceptional properties, including high melting points, superior mechanical toughness, high thermal and electrical conductivity, and excellent chemical stability. Furthermore, their layered architecture provides the possibility to nanoscale into quasi two-dimensional (2D) nanostructures. In general, nanoscaling enhances the accessibility to the intrinsic properties of materials. Over the past decade, our group has established various methods to nanoscale these metal diborides into sheet-like nanostructures. Interestingly, these nanosheets are found to be chemically active and exhibit distinct properties. For example, magnesium diboride (MgB_2) nanosheets were found to exhibit reducing nature, which enables the reduction of gold salts and graphene oxide[1]. In contrast, titanium diboride (TiB_2) based nanosheets demonstrate oxidizing property and are readily reduced by reducing agents such as ascorbic acid[2,3]. Such unique behavior of different metal diborides highlights their inherent chemical activity and their rich potential.

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Structural Stability, Chemical Bonding, and Magnetic Frustration in $TiMOs_2B_2$ Borides

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Abstract

Metal borides provide a versatile platform for exploring how low-dimensional transition-metal substructures control magnetic ordering, electronic structure, and phase stability. In this work, we investigate the $TiMOs_2B_2$ series (M = Cr–Ni), with particular emphasis on the previously missing Cr/Os member, $TiCrOs_2B_2$. The experimentally synthesized $TiCrOs_2B_2$ phase adopts the hexagonal $Ti_{1+x}Os_{2-x}RuB_2$-type structure (P-62m), containing chains of transition-metal triangles coupled to trigonal planar B_4 fragments. Single-crystal and powder X-ray diffraction reveal that $TiCrOs_2B_2$ is close to ideal stoichiometry, whereas other members of the series show stronger deviations associated with excess Os incorporation.

Magnetic measurements show no long-range ordering above 2 K but reveal a remarkably large negative Weiss constant of approximately -4118 K, identifying $TiCrOs_2B_2$ as an exceptionally frustrated magnetic system. Density functional theory calculations, including density of states and projected crystal orbital Hamilton population analyses, were used to rationalize the evolution of bonding and magnetism across the series. The calculations show that strong Os-B, M-B, B-B, M-M, and M-Os interactions stabilize the layered framework, while the position of the Fermi level relative to M-centered antibonding states governs the magnetic response. $TiCrOs_2B_2$ exhibits competing ferro- and antiferromagnetic interactions within Cr-triangle chains, whereas Mn and Fe analogues favor stronger magnetic ordering and Co/Ni members are predicted to be nonmagnetic. These results demonstrate how targeted transition-metal substitution tune stability, bonding, and magnetic frustration in layered borides.

The 2D-to-3D Structural Transition in Boron Nanoclusters and Discovery of Boron Buckminsterfullerene

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Boron, smaller neighbor of carbon, exhibits a unique structural complexity that is driven by its electron deficiency. While small boron nanoclusters exhibit mostly planar or quasi-planar structures, which served as foundational building blocks for 2-dimensional boron sheet namely borophene, the transition to the 3-dimensional bulk-like structures has remained unknown. This presentation combines two landmark discoveries that show 2D-to-3D structural evaluation in boron clusters, and ultimately, highly symmetric molecular cages[1, 2]. Combined reaction kinetics and photoelectron spectroscopy experiments identify B_{46}^- and B_{56}^- nanoclusters to be important transition zones. B_{46}^- reveals a three-dimensional core-shell structure with an inner B_2 core. On the other hand, B_{56}^- marks the first observation of the B_{12} icosahedron core found in bulk boron. These 3D nanoclusters exhibit enhanced reactivity through the chemisorption of CO and C_2H_4. The structural evaluation of boron clusters also reveal the discovery of B_{80} boron buckyball. Spectroscopic data and simulations confirm B_{80} possesses high I_h symmetry. This cage structure is isoelectronic to the well-known C_{60} fullerene. Bonding analyses show that stability is achieved through complex multi-center delocalized bonding network. Together, these findings bridge the gap between 2D boron nanostructures and 3D bulk materials. The identification of the B_{80} buckyball, in particular, paves the way for a new "boron-fullerene chemistry", offering potential applications in hydrogen storage, semiconductor development, and the synthesis of novel molecular solids known as boron fullerites.

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Formation and Characterization of Cu and Ni Nanoparticles Supported on Hydrogen Boride Nanosheets

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Hydrogen boride (HB) nanosheets are two-dimensional materials consisting of a hexagonal boron network with bridging hydrogen atoms.[1] HB nanosheets can reduce specific metal ions without using other reducing agents and support them in a highly dispersed state,[2] making them promising candidates for multi-metallic catalytic applications.[3] However, control over the formation and size of multi-metallic nanoparticles has not yet been studied. In this work, we investigated the formation of Cu and Ni nanoparticles supported on HB nanosheets (Cu-Ni/HB). HB, Cu complexes, and Ni complexes were mixed at different molar ratios (x:y:z) in acetonitrile, yielding Cu_x-Ni_y/HB_z. Transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDX) measurements revealed that the initial amount of metals significantly affected nanoparticle formation. For instance, in Cu_5–Ni_5/HB_{100}, Ni was finely dispersed, whereas Cu tended to agglomerate into submicrometer-sized particles (Fig. 1). This observation was consistent with the X-ray diffraction analysis, in which Cu peaks were observed, while no clear Ni peaks were detected. The effect of the initial metal loading on the formation and dispersion of Cu and Ni nanoparticles will be discussed in the presentation.

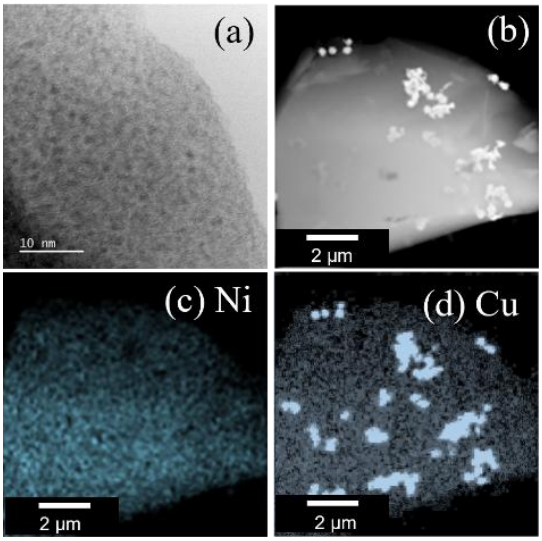

Fig. 1. (a) High-magnification TEM image, (b) dark-field STEM image, and corresponding EDX elemental maps of (c) Ni and (d) Cu for Cu_5–Ni_5/HB_{100}.

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Autonomous Soft X-Ray Absorption Spectroscopy and Machine Learning Analysis of Boron-Based Materials Using the PIONEER System

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Boron-based materials, including hexagonal boron nitride (h-BN), cubic boron nitride (c-BN), and hydrogen boride (HB) sheets, exhibit diverse electronic and structural properties dictated by their distinct bonding configurations. Synchrotron soft X-ray absorption spectroscopy (XAS) is a powerful tool to probe these electronic states; however, conventional manual operations severely limit data throughput, hindering the efficient exploration of spatial phase distributions or local inhomogeneities. To resolve this, we utilized the "PIONEER" (Process Informatics Operando Novel Experiment for Electronic Research) system implemented at NanoTerasu BL08U [1, 2]. This beamline was specifically designed to cover a low-energy soft X-ray region starting from 180 eV, making it uniquely optimized for accessing the boron *K*-edge with high energy resolution and sufficient photon flux.

As shown in Fig. 1, the PIONEER system integrates newly implemented atmospheric and vacuum robotic arms for automated sample handling with our established scanning microscopic XAS chamber [3], enabling 24-hour unattended operation. In this study, we achieved autonomous scanning XAS measurements at the boron *K*-edge across distinct h-BN, c-BN, and HB sheets. The resulting massive XAS dataset, reflecting subtle variations in local coordination and hybridization, was immediately processed through a data-driven machine learning pipeline. Uniform Manifold Approximation and Projection (UMAP) was used for dimensionality reduction to visually map out the electronic variations, followed by k-means clustering for the automated classification and identification of distinct chemical domains without expert bias [4].

In this work, we successfully measured approximately 100 XAS spectra for each boron-based sample via automated scanning, followed by machine learning analysis to visualize the spatial distribution of their electronic states. This combination of focused synchrotron soft X-ray scanning and data-driven machine learning analysis significantly accelerates the research and development of boron-based materials by enabling high-throughput, comprehensive characterization of their complex electronic properties. In the presentation, we will discuss the details of these observed electronic states and the chemical domains identified within the advanced boron-based materials.

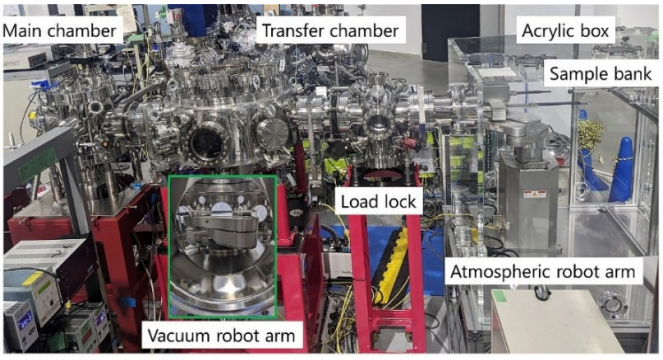

Figure 1. Overview of the developed "PIONEER" system.

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Boron Carbide-Based Ceramics: Effects of Isotopic Abundance, Microstructure, ZrB_2 Addition, and Impurities

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Boron carbide is known for its complex structure and composition-dependent thermal conductivity. In this work, we investigate the thermal conductivity of boron carbide-based ceramics prepared from natural and ^{11}B-enriched boron carbide powders, containing ZrB_2 as an additive and Fe as an unavoidable impurity, with variations in microstructure developed during processing. The choice of ^{11}B isotope and zirconium is motivated by their favorable nuclear properties: ^{11}B has a low neutron absorption cross-section and good neutron reflection capability, while zirconium also exhibits low neutron capture and high radiation resistance. Such properties are of interest for potential applications in space technology, nuclear engineering, and other radiation-intensive environments where thermal management and neutron control are essential. The materials were prepared by introducing zirconium in the form of zirconium oxide via planetary milling with zirconia balls, ensuring homogeneous distribution within the boron carbide matrix. Subsequent hot pressing in vacuum at 2100°C yielded high-density ceramics (relative density 98–100%), where the main phase remained is boron carbide, while ZrB_2 formed as an additive up to 3 wt.%. The fabricated ceramics were characterized by thermal conductivity measurements, scanning electron microscopy, chemical analysis (boron, iron, zirconium, and other elements), as well as by determination of relative density, dynamic and static microhardness, Young's modulus, and other properties. This allowed us to examine correlations between thermal conductivity and material parameters such as phase composition, density, microstructural features, and impurities. The results demonstrate the sensitivity of heat conduction in boron carbide to multiple, simultaneously acting factors. This study highlights the importance of careful control over processing routes and composition when interpreting thermal conductivity data in this system.

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Synthesis of a new diboraanthracene diphosphine ligand and its Ni chemistry

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The synthesis and characterization of a new 9,10-diboraanthracene (DBA) framework with two tethered trialkylphosphine ligands (B_2P_2) and its Ni(0) complex is reported. The strongly donating ligands allow for stabilization of a Ni(I) state, as evidenced by cyclic voltammetry. The electron withdrawing DBA unit stabilized the reduced Ni(0) form via backbonding while the Ni(I) state is stabilized by the strongly donating phosphines. Current work seeks to explore this DBA-based complex to target its reactivity with small-molecule substrates such as H_2, CO_2, and small organic carbonyls.

Highly Conductive PN Cages

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Destructive Quantum Interference (DQI) is a prevalent phenomenon in molecular electronics, dictating transport behavior in σ-conjugated manifolds[1]. To date, these effects have been primarily characterized in silicon-based backbones, leaving the transport properties of broader p-block frameworks largely under-explored. In this work, we employ an inert scanning tunneling microscope-break junction (STM-BJ) approach to study the single-molecule conductance of sensitive Phosphorus-Nitrogen (PN) cages synthesized by the Chitnis group. Contrary to established trends in silicon-based σ-conjugated systems, we find that these cages bypass DQI to exhibit high conductance. Computational analysis using Density Functional Theory and Non-Equilibrium Green's Functions (DFT-NEGF) was utilized to elucidate the electronic origins of this enhanced transmission. These results establish PN cages as a new class of high-conductance p-block molecular junctions.

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Enumeration for Mapping Configurational Landscapes in Al-V and B-C

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We present a full enumeration strategy for mapping the configurational landscape with symmetry-distinct candidate structures within a defined composition, cell size, and structural motif, followed by first-principles evaluation of their relative stability and electronic excitations. Applying this to Al-V, we have identified previously unexplored low-energy structures and modeled the free energy of the body-centered solid solution. We now extend the same framework to the B-C system, where preliminary results indicate a possible new ground state and several low-energy candidates. To account for the cell-size dependence inherent to enumeration, we incorporate a finite-size correction into the free-energy model.

Vacuum-Thermal Exfoliation of Graphene Oxide–Boric Acid (GO–BA) Complexes and Phase Transformation of Obtained Composites in the Temperature Range of 100–1500°C

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Composites obtained from the Graphene Oxide-Boric Acid (GO–BA) system have a wide range of applications, including supercapacitors, batteries, sensors and membrane fabrication, spintronics, wastewater treatment, biomedicine, fire-resistant coatings, and the development of flame-retardant composites and etc. BA forms B–O–C linkages between graphene oxide layers, resulting in the formation of three-dimensional (3D) structured composites characterized by high mechanical strength and enhanced adhesion properties [1]. It has been established that mixing a GO suspension with an aqueous solution of BA at room temperature induces intermolecular interactions between the components, leading to an increase in the hydrodynamic diameter of GO from 250–400 nm to 600–700 nm. The concentration of BA was maintained within the range of 5–20 wt.% relative to the mass of GO. The ζ-potential of particles in the GO suspension was found to be −58 to −61 mV, whereas in the GO–BA suspension it decreased to −43 to −46 mV. In many cases, for the fabrication of specific types of materials, it is preferable to prepare graphene oxide–boron compound composites in the form of ultradispersed powders rather than films. Powdered rGO–HBO_2 composites were obtained from elastic GO–BA films by their vacuum-thermal exfoliation at 160 °C. At the same temperature, under either an inert atmosphere or in air, the films retain their geometric shape without noticeable deformation. As a result of exfoliation, the mass loss of the films reached 44–48%. The particle size of the resulting powder ranged from 1370 to 1547 nm, while the ζ-potential values were between −20 and −21 mV. In contrast, vacuum-thermally exfoliated GO samples exhibited particle sizes 768–788 nm and ζ-potential values −37 to −38 mV. GO-BA complexses undergo the following transformations with increasing temperature: GO–BA → rGO–HBO_2 (160°C) → rGO–B_2O_3 (300-500°C) → G–B_2O_3–B_4C (1500°C). The phase transformation scheme was established based on XRD analysis.

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Importance of boron in the stabilization of full Heusler- and B2-Type (CsCl) Structures in $Mn_{2-x-y}Al_xRuB_y$ solid solution

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Abstract

In attempts to synthesize the predicted quaternary phase "$AlMn_2RuB_3$", new Heusler- and B2-type (CsCl) structures in the $Mn_{2-x-y}RuAl_xB_y$ solid solutions were obtained instead. Rietveld refinements of the powder X-ray diffraction data show that the presence of boron helps in obtaining single-phase products. However, increasing boron also changes the structure from Heusler to B2 (CsCl) structure. For instance, single phases $Mn_{1.5}RuAl_{0.5}B$ and $MnRuAl_{1.5}B_{0.5}$ were obtained with the B-rich phase crystallizing in the B2-type structure (CsCl-type, space group no. 221, $Pm\bar{3}m$) while the B-poor phase adopts the conventional $L2_1$ Heusler structure (space group no. 225, $Fm\bar{3}m$). Scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS) reveals a homogeneous microstructure with uniform elemental distribution and no detectable secondary phases, confirming the high phase purity inferred from diffraction analysis.

Thermal Dehydrogenation-Induced Magnesium Dispersion on Boron-Based Nanosheets

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Two-dimensional nanosheets can serve as platforms for dispersing metal species owing to their large surface area and accessible surfaces. Hydrogen boride (HB) nanosheets are particularly attractive boron-based 2D materials, offering both nanoscale boron frameworks and reactive hydrogen-related sites.[1] In this study, Mg-dispersed boron nanosheets were synthesized by heating HB nanosheets with ball-milled MgH_2 at 550 °C. Scanning transmission electron microscopy (STEM) and energy dispersive X-ray spectroscopy (EDS) analyses confirmed uniform Mg dispersion and suppression of Mg aggregation (Figure 1). Temperature-dependent X-ray diffraction patterns suggested that Mg diffused after H_2 release from HB and MgH_2, where it became trapped at hydrogen vacancies in the HB nanosheets. X-ray photoelectron spectroscopy and density functional theory results further indicated that the electronic states of Mg and B were similar to those in MgB_2, supporting the formation of Mg–B bonding. These findings demonstrate that HB nanosheets can act as a boron-based two-dimensional platform for stabilizing highly dispersed Mg species.

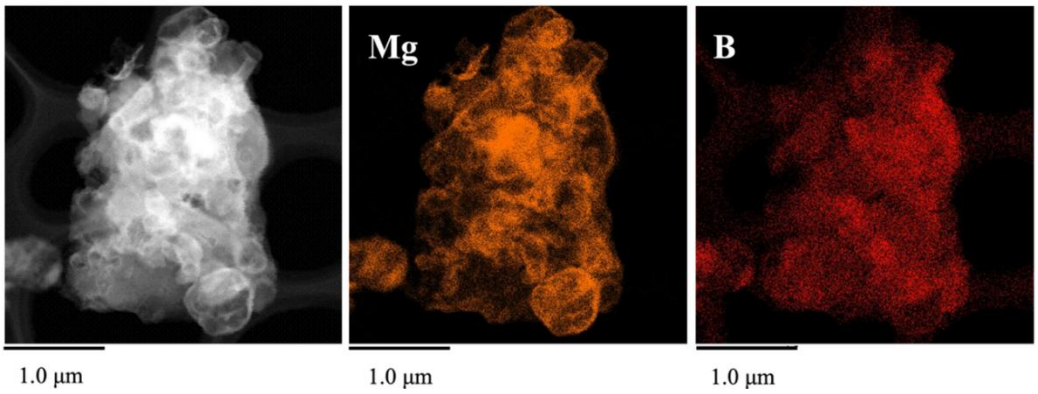

Figure 1. STEM and EDS mapping of highly dispersed Mg on boron nanosheets.

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Transformations of Small Boron Clusters According to Semiempirical Diatomic Molecular Model

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Small clusters consisting solely of boron atoms, which prefer (quasi)planar structures, can be considered building blocks for growing 2D boron-based materials[1] promising in many modern advanced technologies. Their ground-state parameters—specific bonding energy, bonds length, zero-point vibration frequency, etc.—were estimated within the framework of a semiempirical diatomic molecule model[2,3] taking into account the influence of nonzero static atomic charges[4,5] characteristic even of clusters of identical atoms due to their finite size. Here, based on these results, the reaction energies are obtained for the transformations $B_m^k + B_n^l \rightarrow B_\mu^\kappa + B_\nu^\lambda$, where m, n, μ, $\nu = 0, 1, 2, \ldots, 20$ are the numbers of boron atoms in the clusters for $m + n$, $\mu + \nu \leq 20$, and k, l, κ, $\lambda = -1, 0, +1$ are their charge numbers for $|k + l|$, $|\kappa + \lambda| \leq 1$. For 5 small boron clusters (B_5, B_8, B_{11}, B_{14}, and B_{17}), which are expected to have a planar asymmetric shape[6] with nonzero electric dipole moments in the ground state, dipole–dipole interactions will also be considered.

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Ternary Li-Ni-B compounds as promising catalysts for water splitting in alkaline media

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Intermetallic borides display a wide range of crystal structures, bonding motifs, and functional properties. Borides can be found as state-of-the-art materials in contexts such as permanent magnetism, superconductivity, magnetocaloric effect, and superhardness. [1–3] Most transition metal borides are metallic and are resistant to degradation in extremely acidic or alkaline environments.[3] This makes them ideal candidates for electrocatalysts for water splitting, which occurs as two half-reactions: oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). At present, the primary catalysts for both reactions contain critical platinum-group metals.[3,4]

While binary borides of first-row transition metals have been extensively explored for OER/HER activity, the class of ternary borides containing both an alkali metal and a first-row transition metal have not yet been studied. The relative scarcity of such phases may be due in part to the synthetic difficulties associated with obtaining them from direct reactions of the constituent elements.[5] In this work, we demonstrate the efficient synthesis of several phases in the Li-Ni-B ternary system using the hydride route, where the alkali metal is replaced by its salt-like hydride to enable better mixing and faster reactions.[6] We then show how post-synthetic ball milling to reduce particle size and increase the amount of exposed surface is crucial to realize the full electrocatalytic activity of these materials. The native Li-Ni-B compounds likely serve as pre-catalysts that generate an active layer of transition metal oxyhydroxides upon application of electric potential; the resulting surface states are investigated post-catalysis by XPS and TEM. The composition-structure relationship in the context of catalyst stability and activity for both alkaline OER and alkaline HER processes will be discussed for this family of Li-Ni-B compounds.

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Effect of Catalyst Surface Hydrophilicity on Oxygen Evolution Reaction

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Clean hydrogen production via water electrolysis is crucial for sustainable energy systems, but its efficiency is hindered by the sluggish oxygen evolution reaction (OER), requiring high-performance catalysts. Rhombohedral boron monosulfide (r-BS), composed of earth-abundant boron and sulfur, has emerged as a promising OER catalyst owing to its high activity and stability[1,2]. In our previous study[3], we found that the OER activity of r-BS strongly depends on the surface wettability of carbon supports, where more hydrophilic supports such as graphene enhanced catalytic performance compared with hydrophobic multi-walled carbon nanotude (MWCNT) (Figure 1).

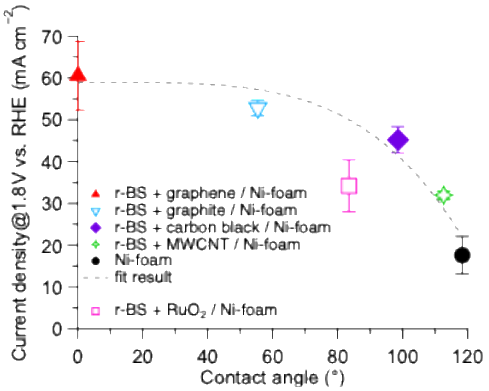

Figure 1. Influence of catalyst surface hydrophilicity on OER performance.

Here, we further investigate the role of interfacial hydrophilicity by introducing a superhydrophilic coating based on sputter-deposited 316 stainless steel[4] onto r-BS + carbon-material electrodes. The coated electrodes were evaluated in 1 M KOH using linear sweep voltammetry (LSV) measurements, and their surface wettability was analyzed by contact angle measurements. The hydrophilic coating markedly improved electrode wettability regardless of the carbon support and consistently enhanced OER activity. Notably, coated r-BS electrodes exhibited higher performance than RuO_2, suggesting that improved bubble release at the electrode interface contribute to the enhanced activity. These results indicate that interfacial wettability is a key factor governing OER performance. The relationship between surface hydrophilicity and catalytic activity in r-BS-based OER electrodes will be discussed.

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Interlayer Hydrogen Spacing Regulates the Formation of Molecular Hydrogen in Hydrogen Boride Nanosheets

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Hydrogen carriers that enable efficient transport and on-demand release of H_2 are crucial for practical hydrogen-based energy systems. Hydrogen boride (HB) nanosheets, composed of boron and hydrogen in a 1:1 stoichiometric ratio, are promising safe and lightweight hydrogen carriers owing to their high gravimetric hydrogen density (8.5 wt %).[1] However, the mechanism of the multimodal H_2 desorption upon heating remains unclear. Here, we show that the interlayer H···H distances ($d_{H\cdots H}$) govern the multimodal desorption of H_2 especially in the lower-temperature range (Figure 1).[2] Infrared spectroscopy and temperature-programmed desorption (TPD) measurements revealed the occurrence of hydrogen depletion without changes in bonding configuration. The first to third nearest $d_{H\cdots H}$, along with the numbers of the corresponding H···H pairs, were systematically calculated for four possible interlayer stacking types. The calculated pair distribution closely matched the experimental desorption profile, indicating that lower-temperature multimodal H_2 desorption is governed by $d_{H\cdots H}$ distributions.

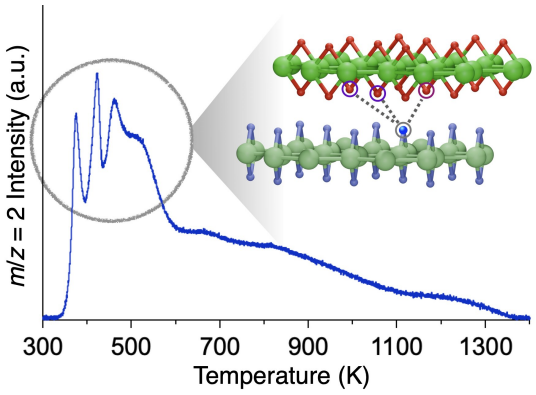

Figure 1. A representative multimodal H_2-TPD profile of HB nanosheets with a schematic illustration of interlayer H···H distances.

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MOF-Inspired Materials Design: Structure Building Block Principles in Metal-rich Borides

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Understanding the structure-building principles for extended solids allows us to predict new crystal structures and enables materials-by-design. In this work, we present an intuitive classification of 16 different structure types that represent over 50 different ternary and quaternary metal borides based on a shared building unit. We lay out the structure building principles such as unit cell twinning and different tessellations while also explaining the occurrence of low-dimensional motifs of magnetic elements and the size of B_n-fragments in these structures with respect to the constituent metals. We find electronic conditions for stability and predict new, yet to be discovered boride crystal structures containing novel low-dimensional motifs of magnetic elements and B_n units. Last, we study their electronic and magnetic properties by density functional theory.

One-Step Synthesis of Layered Borophene Oxide Thin Films Exhibiting a Thermotropic Liquid-Crystalline Phase Transition

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Layered borophene oxide (BoL, $B_{4.27}KO_3$) has been reported as the first inorganic liquid crystal (LC) that exhibits thermotropic behavior, with a phase transition at 120°C [1,2]. To date, BoL has been obtained only in a bulk polycrystalline form by a liquid-phase reaction of KBH_4 in acetonitrile (MeCN); however, thin-film fabrication of BoL is essential for its future inorganic-LC device applications. Here, we report a room-temperature, one-step synthesis of BoL thin films via continuous-wave infrared (CW-IR) laser deposition of KBH_4 under an MeCN vapor (10 mTorr).

The out-of-plane XRD patterns of a film prepared under high vacuum showed only KBH_4-derived peaks (Fig.(a)). By contrast, a film prepared under MeCN vapor showed dominant peaks assigned to BoL (00*l*) reflections, in additions to the KBH_4-derived peaks. This result indicates the formation of layered BoL thin films with an out-of-plane periodicity consistent with that of bulk BoL. When the BoL thin film was heated to 60–70°C, these BoL (00*l*) reflections disappeared, and polarized optical microscope (POM) observation revealed a distinct change in optical texture (Fig.(b)). Raman and IR spectra further showed that the spectral features associated with B–OH bonds disappeared across this transition. Together, these results suggest that the thin film undergoes the similar dehydration-driven LC phase transition, to that reported for bulk BoL [2]. In fact, the transition temperature is approximately 50-60°C, much lower than that of bulk BoL, which is a remarkable advantage for BoL-based inorganic-LC device applications.

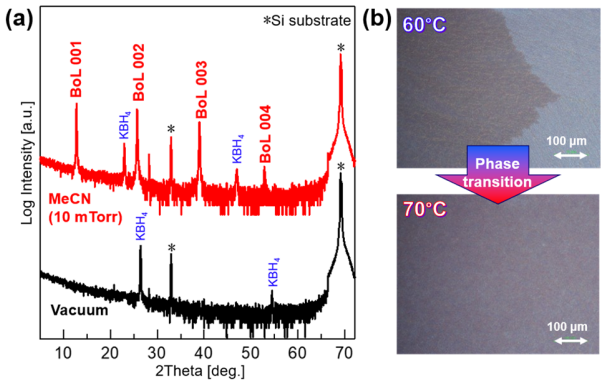

Fig.(a) Out-of-plane 2θ-θ XRD patterns of films deposited on Si (100) substrates under MeCN vapor (10 mTorr; red) and under vacuum (black). (b)POM images of the BoL thin film during heating.

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Synthesis of Sodium-Doped Hydrogen Boride toward Enhanced Hydrogen Adsorption Performance

Shohei Shimozato[1], Kosuke Takeshita[1], Natsumi Noguchi[1], Miwa Hikichi[1], Shin-ichi Ito[1], Osamu Oki[1], Kazuki Yamaguchi[2], Iwao Matsuda[2], Shin-ichi Orimo[3], Takahiro Kondo[1,3,4*]

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The realization of hydrogen society requires hydrogen (H_2) adsorbents that enable H_2 uptake and release under near-ambient conditions and exhibit high gravimetric H_2 density. Hydrogen Boride (HB) nanosheets are lightweight two-dimensional materials composed of positively charged hydrogen and negatively charged boron.[1] Previous theoretical studies predicted that the Na-doped HB monolayers exhibit the high H_2 adsorption property under near-ambient conditions. However, the synthesis of Na-doped HB and their H_2 adsorption property have not yet been demonstrated experimentally.[2] In this study, we developed a synthetic method to fabricate Na-doped HB via an ion-exchange method based on acid-base neutralization reaction.

Na-doped HB was prepared through the reaction between an acidic HB aqueous dispersion and a basic sodium hydroxide (NaOH) aqueous solution (Fig. 1). X-ray photoelectron spectroscopy (XPS) of the sample showed the Na 1s peak and the negatively charged B peak, indicating that Na was introduced by the substitution of H in HB. Fourier Transform Infrared Spectroscopy (FT-IR) spectra showed a change in peak shape near 1350 cm^{-1}, assigned to the in-plane B–H–B stretching vibration. Detailed peak separation analysis revealed the formation of compressed and stretched B–H–B groups, which is consistent with the theoretically predicted framework of Na-doped HB.[2] These structural characterizations demonstrate the successful synthesis of Na-doped HB. H_2 adsorption measurments showed that H_2 uptake was 0.092 wt% for HB and 0.17 wt% for Na-doped HB (298 K, 11.4 MPa), respectively. This indicates that Na doping in HB enhanced H_2 adsorption property.

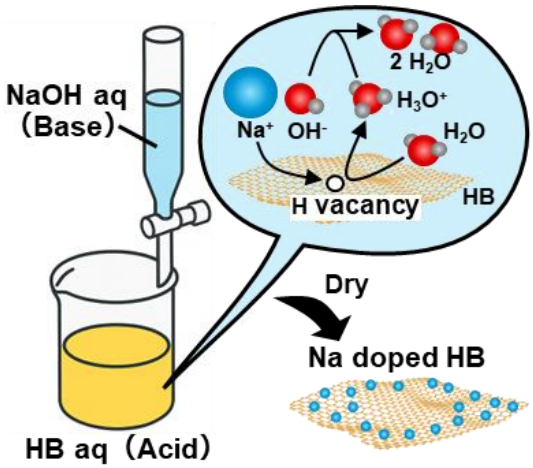

Fig.1 Synthesis Method of Na-doped HB

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Electrochemical Activation and Oxidative Stability of Diborides for Hydrogen Evolution

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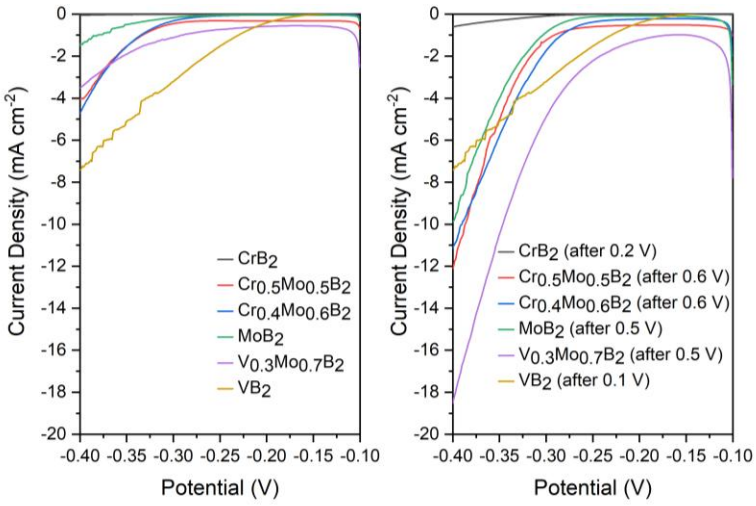
Abstract:

Transition-metal diborides are promising non-noble-metal electrocatalysts whose activity is strongly influenced by metal composition, vacancies, and metal-boron bonding. Recent studies of V-Mo and Cr-Mo diborides have established that metal vacancies, metal-boron bonding, and composition-dependent structural changes play important roles in determining HER activity. However, the influence of oxidative electrochemical pretreatment on the catalytic behavior and structural integrity of these materials remains largely unexplored.

Here, we investigate the electrochemical response of a systematic series of diborides comprising CrB_2, $Cr_{0.5}Mo_{0.5}B_2$, $Cr_{0.4}Mo_{0.6}B_2$, MoB_2, $V_{0.3}Mo_{0.7}B_2$, and VB_2. Raman spectroscopy was used to establish the initial vibrational signatures of each material, followed by controlled chronoamperometry and HER measurements. Remarkably, oxidative electrochemical pretreatment substantially enhances HER activity across the entire series, demonstrating that the catalytic state of these borides depends strongly on their electrochemical history. Despite this common activation response, the potential-dependent behavior is highly composition-specific. $Cr_{0.5}Mo_{0.5}B_2$, and $Cr_{0.4}Mo_{0.6}B_2$ retain their enhanced activity following oxidative treatment up to 1.0 V vs RHE, whereas MoB_2 and $V_{0.3}Mo_{0.7}B_2$ begin to lose activity above approximately 0.5 V, coincident with increasing oxidative currents in chronoamperograms. VB_2 exhibits the greatest oxidative susceptibility, with activity decreasing following treatment above only 0.1 V. In contrast, the initially least-active CrB_2 undergoes an activation maximum near 0.2 V before subsequent activity loss.



These results demonstrate that oxidative activation and degradation are strongly dependent on metal composition and reveal a previously unrecognized distinction between catalytic activation and electrochemical instability in transition-metal diborides. The findings provide a framework for correlating composition, electrochemical history, and structural evolution in boride electrocatalysts.

Stabilization of the $L2_1$ Heusler Structure in a New Ternary Compound Mn_2RuIn

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Abstract

The compositional flexibility of Heusler compounds provides an effective approach for tuning their physical properties through main-group element substitutions. Herein, we report on the successful synthesis and structural characterization of the ternary Heusler compound Mn_2RuIn. Polycrystalline Mn_2RuIn samples were synthesized via a conventional solid-state reaction followed by annealing, yielding a single-phase material. Powder X-ray diffraction coupled with Rietveld refinement confirms that Mn_2RuIn crystallizes in the $L2_1$ Heusler structure, indicating that substitution of Ge by In preserves the ordered cubic framework of the parent Mn_2RuGe compound. In the refined structural model, In fully occupies the 4*a* crystallographic site, replacing Ge, while Mn and Ru occupy the remaining Wyckoff positions characteristic of the $L2_1$ structure. Scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS) reveals a homogeneous microstructure with uniform elemental distribution and no detectable secondary phases, confirming the high phase purity inferred from diffraction analysis. The retention of the $L2_1$ structure following complete Ge-to-In substitution demonstrates the structural robustness of this Ru-based Heusler family and highlights the compatibility of In with the ordered Heusler framework. These findings establish Mn_2RuIn as a new member of the Ru-based ternary Heusler family and provide a structural foundation for future investigations of its electronic, magnetic, and transport properties.

Electronic Structure and Spectroscopic Properties of β-Boron and Subhydride β-Boron: A First-Principles Study

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β-rhombohedral boron (β-boron) and its subhydride form, $B_{104.67}H_3$, have attracted attention because of their unusual structural and electronic properties [1, 2]. Experimental studies have suggested that the lattice expansion and contraction observed in β-boron may be related to hydrogen incorporation and that subhydride β-boron could potentially function as a photo-switchable hydrogen storage material [3–5]. In our previous studies presented at ISBB2024, we investigated the stability of hydrogen sites and hydrogen content in subhydride β-boron using first-principles calculations and estimated the hydrogen concentration through comparison with experimentally observed lattice expansion.

In this study, we further examine the electronic structure, optical response, and core-level spectroscopic properties of β-boron and subhydride β-boron in order to gain insight into the hydrogen desorption mechanism. First-principles calculations were performed using the VASP code [6]. Optical responses, including absorption spectra, were evaluated within the independent-particle approximation based on electronic transitions from occupied to unoccupied states. In addition, B K-edge XANES spectra were calculated using the core-hole approach to investigate the relationship between local atomic environments and unoccupied electronic states. Preliminary XANES calculations suggest possible site-dependent variations in the spectral features of β-boron-based systems. However, further examination of the core-hole-induced charge redistribution and its influence on the local electronic structure is necessary for quantitative interpretation.

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References

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Defect-Engineered β-B-derived nanosheets and Heterointerfaces for Efficient Electrochemical Water Splitting

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The development of boron-based two-dimensional materials has attracted increasing attention owing to their distinctive electronic structure and potential in electrocatalytic energy conversion. Despite extensive theoretical interest in borophene, the fabrication of stable, free-standing crystalline phases remains challenging. Here, we investigate an alternative route based on defect induced cleavage of β-rhombohedral boron to obtain ultrathin borophene-like nanoflakes. The proposed top-down methodology (ball-milling, modified Hummers method, ultrasound assisted liquid phase exfoliation) utilizes the presence of landscape of defects such as line and planar defects within the β-B framework to induce selective structural disintegration. This transformation results in the formation of β-B-derived nanosheets characterized by a high density of edge sites, amorphous regions, and partially oxidized surface domains. Such structural heterogeneity creates a large population of catalytically accessible centers capable of promoting both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). To further optimize charge-transfer kinetics and active-site utilization, the boron-derived nanoflakes were combined with transition-metal-containing phases, yielding hybrid heterostructures with improved interfacial electronic communication. Comprehensive structural, spectroscopic, and electrochemical analyses demonstrate that catalytic efficiency is governed by the interplay between defect concentration, surface reconstruction processes, and heterointerface formation. The results highlight defect-rich boron nanomaterials as a versatile platform for the rational design of next-generation bifunctional electrocatalysts for sustainable hydrogen production.