Nano and 2D Materials
Room Naupaka Salon 4 - Session NM2-TuE

2D Materials Based on Carbon and Boron
Moderator: Akitoshi Shiotari, Fritz-Haber Institute

7:40pm **NM2-TuE-7 First-Principles Study of Adsorption and Reaction on the Hydrogen Boride Sheet***, Ikutaro Hamada,* Osaka University, Japan **INVITED**

The hydrogen boride (HB) sheet [1] is a newly synthesized two-dimensional material composed of hydrogen and boron atoms with their ratio of 1:1. The HB sheet has been attracted increasing attention, not only because of its high gravimetric hydrogen content as a hydrogen storage material and its ability to release hydrogen through light [2] and electrochemical [3] means, but also due to its catalytic activities [4]. Furthermore, the HB sheet has been shown to be chemically stable against water [5], unlike many boron hydrides that undergo hydrolysis reactions. The stability is a fascinating considering the practical application of the HB sheet. However, the molecular and mechanistic details of the chemical processes occurring on the HB sheet have yet to be fully addressed. In this talk, I will discuss the electronic and structural properties of the HB sheet [5], as well as the adsorption and reaction on the HB sheet based on our density functional theory calculations. Special emphasis is placed on the interaction with water molecules, and the mechanism of the stability of the HB sheet against water will be discussed [6,7].

References:

[1] H. Nishio, *et al*., J. Am. Chem. Soc. **139**, 13761 (2017).

[2] R. Kawamura, *et al*., Nat. Commun. **10**, 4880 (2019).

[3] S. Kawamura, *et al*., Small **20**, 2310239 (2024).

[4] T. Goto, *et al*., Commun. Chem. **5**, 118 (2022).

[5] L. T. Ta, Y. Morikawa, and I. Hamada, J. Phys. Condens. Matter **35**, 435002 (2023).

[6] K. I. M. Rojas, *et al*., Commun. Mater. **2**, 81 (2021).

[7] K. I. M. Rojas, Y. Morikawa, and I. Hamada (submitted).

8:20pm **NM2-TuE-9 N-doped Graphene Synthesis through Nitrogen Ion Irradiation***, Zbynek Novotny,* Pacific Northwest National Laboratory*; Buddhika Alupothe Gedara, Prescott Evans, Zdenek Dohnalek,* PNNL

Hydrogen (H_2) is one of the most promising clean and renewable energy carriers. Nevertheless, the ability to store and transport hydrogen is inefficient due to the low volumetric densities. Nitrogen-doped graphene (Gr) has been identified as a potential material for H_2 storage. We study the growth of Gr on a Ru(0001) surface by chemical vapor deposition (CVD) of pyridine (H_5C_5N) and N-doping through N_2^+ ion irradiation using scanning tunneling microscopy (STM) and x-ray photoelectron spectroscopy (XPS). A high-quality Gr film with low N densities was obtained by pyridine CVD on Ru(0001) at 1100 K. Higher concentrations of N-dopants were introduced on the Gr/Ru(0001) through low-energy N_2^+ irradiation at 100 eV. Nitrogen can be embedded in the Gr lattice preferentially in two configurations, namely graphitic N (N substituted in the C lattice) and pyridinic N (substitutional N next to a C vacancy). Atomically-resolved STM images of graphitic and pyridinic-N defects demonstrate their preferential locations within the Gr Moiré. XPS shows that coverage of up to 3.9% of pyridinic-N and 2.3% of graphitic N can be embedded into the high-quality Gr film using N_2^+irradiation at room temperature, indicating a preferential formation of pyridinic N over graphitic N. Only graphitic N was observed upon annealing the ion-irradiated Gr/Ru(0001) to 1063 K, revealing higher thermal stability of graphitic N over pyridinic N. Our current efforts center on the adsorption studies of atomic hydrogen, its interactions with N dopants, and thermally induced diffusion.

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