van der Waals density functional study of simple molecules adsorption on borophene

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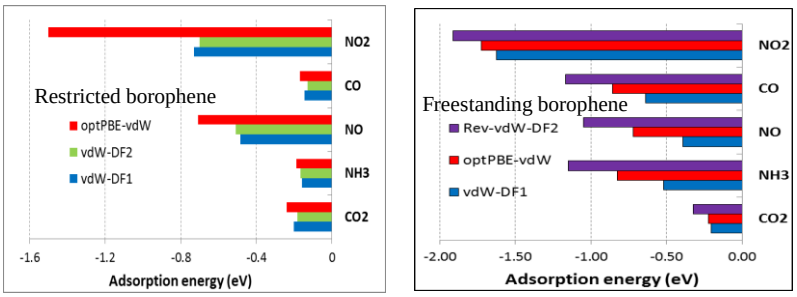
Recently, β_{12} borophene has been received great attention due to its potential properties to be applied in electronic devices such as possessing spin gapless Dirac cone, rich band structure, and high Young's modulus, etc. However, the interaction between common gases and β_{12} borophene has been still remaining ambiguously.

To provide an insight into adsorption behavior of borophene, we study the interactions of β_{12} borophene towards five hazardous gases namely CO, NO, NH_3, NO_2, and CO_2 using van der Waals density functionals method. Among considered gases, CO_2 is physisorbed meanwhile other gases have chemically bonding with β_{12} borophene. Notably, NO_2 exhibits its superior interaction with borophene, suggesting the potential of borophene in sensing or capturing this gas. Besides, we take into account the effects of vdW correlation models and constraint of geometry. We found that the adsorption energies given by vdW-DFs increase as the order of vdW-DF1≈vdW-DF2 < optPBE-vdW < rev-vdW-DF2 and CO and NH_3 are likely to be susceptible with the constraint on geometry of borophene.



In this presentation, we also provide the details of orbital hybridization between atomic orbitals of boron and molecular orbitals of molecules by COOP, PDOS and vibrational analysis; thereby, elucidating the adsorption mechanism, the origin of preferable adsorption site and redshift of molecules' stretching modes. The results are expected to benefit experiments related to this topic in very near future.