Theoretical Studies on Novel Physical Properties Arising from Many-Body Interaction

MINAMITANI, Emi
Associate Professor
eminamitani@ims.ac.jp

Quantum many-body interaction is a source of novel physical properties in the condensed matters. In our group, we develop theoretical methods by combining quantum field theory and density functional theory, and carry out collaborative research with experimental groups. As specific targets, we focus on magnetism in nanostructure and energy dissipation.

For magnetism in nanostructure, we are interested in the Kondo effect and spin–orbit interaction. The Kondo effect arises from the interaction between the localized spin and conduction electrons, which forms a characteristic many-body state so called the Kondo singlet state. The spin–orbit interaction originating from relativistic effect constrains the direction of magnetic moment to specific direction. We investigate the possibility of novel physical phenomena induced by these interactions in the nanostructure and molecules on surfaces.

For energy dissipation, we focus on the effect of electron–phonon interaction. The electron–phonon interaction is one of the most fundamental interactions in the condensed matter physics, and the quantitative evaluation in realistic materials is highly demanding. We adopt the ab-initio calculation to analyze the signal of electron–phonon coupling in surface spectroscopy and thermal properties in various kind of solids.

Selected Publications
1. Superconductivity in Chemically Doped 2D Materials

Layered materials have been investigated for a long time owing to their tunable features, which enable various applications. Amongst them, superconductivity has recently attracted considerable attention. Although several types of 2D superconductors have been experimentally and/or theoretically investigated, most of them are metallic/semimetallic materials, such as metal atomic layers on semiconductor surfaces, layered materials such as FeSe and NbSe₂, and electron-doped graphene. The other class of 2D superconductors is doped 2D semiconductors or insulators.

We focused on hexagonal boron nitride (h-BN) as a candidate for a 2D superconductor. Bulk h-BN has a wide bandgap of approximately 6 eV, and it exists in the monolayer form. Although the application of h-BN as an inert and atomically flat insulating layer to realize novel 2D-material-based electronics has been widely investigated, its possibility as a superconductor has been untapped until recently. In our previous study, we reported that a Li-intercalated h-BN bilayer became a phonon-induced superconductor with a \( T_c \) of up to 25 K, thereby indicating that both the phonon properties and electron–phonon coupling (EPC) in doped h-BN are appropriate for realizing superconductivity. ¹ However, the fabrication of a superconducting Li-intercalated h-BN bilayer is experimentally challenging, as the stacking order of the h-BN sheets must differ from that of the original bulk structure to attain a high \( T_c \). To seek a promising candidate for an h-BN-based superconductor with a more experimentally feasible structure than the bilayer structure, we investigated the properties of doped monolayer h-BN by using ab-initio calculation of electron–phonon interaction.

Consequently, we reveal that Sr- and Ba-doped monolayer h-BN and Ca-doped monolayer h-BN with 3.5% tensile strain are energetically stable and become superconductors. ² The estimated \( T_{cs} \) from McMillan–Allen–Dynes formula are approximately 5.83, 1.53, and 10.7 K, respectively. Interestingly, the \( T_{cs} \) for the Ca-, Sr-, and Ba doped graphene are lower than 0.5K.

\[ T_{cs} \]

\[ \lambda \]

The enhancement in \( \lambda \) around the \( \Gamma \) point in the Ca-doped h-BN is attributed to the spatial distribution of the wavefunction of the electronic states induced by the lower symmetry compared to the graphene case. These results indicate that instead of tuning the interlayer state, reducing the symmetry and introducing strong adsorbate–substrate interactions are alternative strategies to increase the \( T_c \) of doped 2D semiconductors/insulators.

Other Ongoing Projects:
- Geometric Spin–Orbit Coupling and Chirality-Induced Spin Selectivity
- Ab-Initio Calculation of Heat Generation in Semiconductors

Figure 2. Electronic band dispersions and DOS for doped h-BN and graphene.

Figure 3. Fermi surfaces and k-resolved EPC projected on Fermi surface in doped h-BN and graphene.

References