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

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Professional Employment
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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.

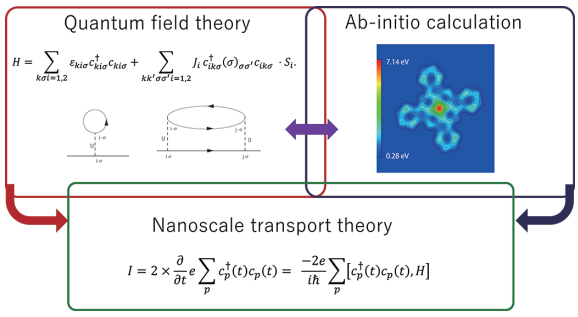

Figure 1. Schematic image of the theoretical method developed in our group.

Selected Publications

- E. Minamitani, N. Tsukahara, D. Matsunaka, Y. Kim, N. Takagi and M. Kawai, "Symmetry-Driven Novel Kondo Effect in a Molecule," *Phys. Rev. Lett.* **109**, 086602 (2012).
- E. Minamitani, R. Arafune, N. Tsukahara, Y. Ohda, S. Watanabe, M. Kawai, H. Ueba and N. Takagi, "Surface Phonon Excitation on Clean Metal Surfaces in Scanning Tunneling Microscopy," *Phys. Rev. B* **93**, 085411 (2016).
- E. Minamitani, N. Takagi and S. Watanabe, "Model Hamiltonian Approach to the Magnetic Anisotropy of Iron Phthalocyanine at Solid Surfaces," *Phys. Rev. B* **94**, 205402 (2016).
- R. Hiraoka, E. Minamitani, R. Arafune, N. Tsukahara, S. Watanabe, M. Kawai and N. Takagi, "Single-Molecule Quantum Dot as a Kondo Simulator," *Nat. Commun.* **8**, 16012 (2017).
- E. Minamitani, R. Arafune, T. Frederiksen, T. Suzuki, S. M. F. Shahed, T. Kobayashi, N. Endo, H. Fukidome, S. Watanabe and T. Komeda, "Atomic-Scale Characterization of the Interfacial Phonon in Graphene/SiC," *Phys. Rev. B* **96**, 155431 (2017).
- E. Minamitani, M. Ogura and S. Watanabe, "Simulating Lattice Thermal Conductivity in Semiconducting Materials Using High-Dimensional Neural Network Potential," *Appl. Phys. Express* **12**, 095001 (2019).

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 $NbSe_2$, 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.

To clarify the difference between h-BN and graphene, we analysed the electronic band structure depicted in Figure 2. The projection of the DOS from the adsorbate s-orbital onto the electronic-band structures indicated the presence of adsorbate bands that crossed the Fermi level in all systems. These bands correspond to the interlayer state reported in previous studies. In doped graphene systems, the interlayer state is crucial for determining T_c. However, the similarity in the interlayer state between doped graphene and h-BN indicates that the T_c in these systems is governed by other factors. Other than the interlayer states, several bands that originated from h-BN and graphene orbitals crossed the Fermi level.

These band structures around the Fermi level resulted in Fermi surfaces of different shapes and positions, as depicted in Figure 3. In both the h-BN and graphene cases, the Fermi surface around the K point originates from the interlayer state, and those around the Γ point correspond to the band from the h-BN or graphene states. The shape of the Fermi surfaces from the interlayer states resembled each another in both the doped h-BN and graphene cases, except for the size of the pocket.

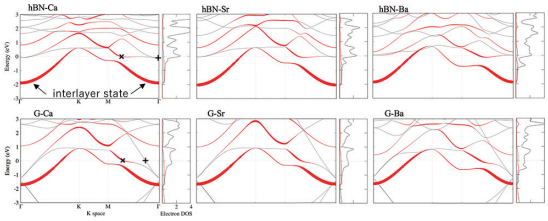

Figure 2. Electronic band dispersions and DOS for doped h-BN and graphene.

However, the shapes of the inner Fermi surfaces around the Γ point between the doped h-BN and graphene cases differed significantly. In the doped h-BN case, the inner Fermi surface exhibited a snowflake-like shape, but it was hexagram-like in the doped graphene case. The projection of the k-resolved EPC (λ_k) shows that the electron–phonon interaction in the inner Fermi surface is crucial for determining T_c. Compared with doped graphene, the doped h-BNs exhibited greater λ_k in general in the Brillouin zone. The most prominent enhancement in λ_k was observed around the Γ point.

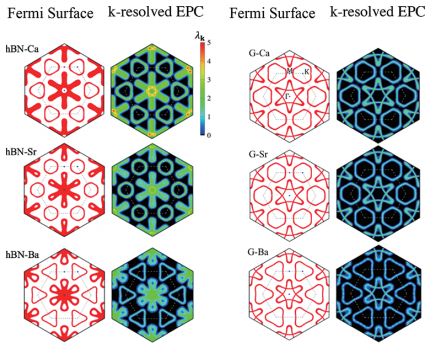

Figure 3. Fermi surfaces and k-resolved EPC projected on Fermi surface in doped h-BN and graphene.

The enhancement in λ_k around the Γ 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

References

1) N. H. Shimada, E. Minamitani and S. Watanabe, *Appl. Phys. Express* **10**, 9 (2017).

2) N. H. Shimada, E. Minamitani and S. Watanabe, *J. Phys.: Condens. Matter* **32**, 435002 (2020).