Road to Realistic Quantum Material Design: Bridges First-Principles and Many-Body Theory

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Quantum material is a material class whose essential properties only can be explained by quantum mechanical effects. The emergent properties of quantum material are crucial for future technology in the 21st Century. For example, superconductivity, magnetism, metal-insulator transition, and topological properties are useful properties of a quantum material for its applications to electronic devices, quantum computers, and electric motors.

In this presentation, I will discuss our roadmap for designing the quantum material to control its emergent quantum properties using computational methods. The realistic description of the quantum materials' properties is possible from the combination of the first-principles method and the many-body method, such as the density functional theory (DFT) and the GW method in combination with the dynamical mean-field theory (DMFT), capturing the strong electronic correlations in quantum materials, beyond the single particle pictures of the electrons. It will be shown that the electronic correlations are essential for electronic structures [1], symmetry breakings [2], and topological properties [3] of quantum materials. In particular, topological superconductivity, a prime candidate for topological quantum computation in iron-based superconductors, will be discussed with the importance of dynamical electronic correlations [3]. From these realistic descriptions, using both advantages of the first-principles methods and the many-body theory, a strategy for the realistic quantum material design using the computational method will be shown to control emergent quantum properties, a central agenda of quantum technology.

[1] **Minjae Kim**[*] et al., Phys. Rev. Lett. 120, 126401 (2018).

[2] S. Hahn[*], B. Sohn[*], **Minjae Kim**[**], C. Kim[**] et al., Phys. Rev. Lett. 127, 256401 (2021)

B. G. Jang[*], **Minjae Kim**[**], Y.-W. Son[**] et al., Phys. Rev. Lett. 130, 136401 (2023)

[3] **Minjae Kim**[*] et al., Phys. Rev. Lett. 132, 136504 (2024).