Design of Topological and Strongly-correlated Materials by Ab initio Calculations

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Abstract: Research on the topological properties of the wave function attracts a great deal of attention [1]. In this seminar, first, we show that electrides are suitable for achieving various topological insulating and topological semimetal phases [2]. In electrides, some electrons reside in the interstitial regions and act as anions to stabilize the structure. Since interstitial electrons have small work function, band inversion around the Fermi level is likely to occur. We find that Sc2C shows nontrivial insulating phase characterized by the π Zak phase. This π Zak phase appears as a surface polarization charge, and we propose that this surface charge is useful for carrier doping by using the electride. We also show the result of electride apatite as a higher-order topological crystalline insulator [3]. We find various topological electrides such as HfBr (quantum spin Hall system), and LaBr (quantum anomalous Hall insulator).

Next, we show the result for the Majorana Fermion. Here, we perform fully non-empirical calculation for the CMM considering superconductivity and surface relaxation, and show that hexagonal close-packed thallium (Tl) has an ideal electronic state that harbors the CMM [4]. The kz = 0 plane corresponds to the topological crystalline insulator. Only one of the two Dirac points is relevant for the gap opening due to the superconducting transition, and the CMM appears at the hinge under the Zeeman field.

If time is left, we also show the material design for the strongly correlated systems such as Cu- and Ni-based superconductors by using constrained RPA and constrained

GW methods.

References:

[1] M.Hirayama, R. Okugawa, and S. Murakami, J. Phys. Soc. Jpn. 87, 041002 (2018). (Review)

[2] M.Hirayama, S. Matsuishi, H. Hosono, and S. Murakami, Phys. Rev. X 8, 031067 (2018).

[3] M.Hirayama, R. Takahashi, S. Matsuishi, H. Hosono, and S. Murakami, submitted.

[4] M. Hirayama, T. Nomoto, and R. Arita, submitted.