

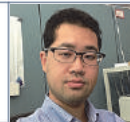
Theoretical Study on Design and Control over Topological Materials

Keywords: Topological insulator, Topological semimetal, Electronic structure calculation

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Background

- Topological insulators/semimetals as a frontier of material science
- Expectation for new functionalities of matter using characteristic feature of unconventional insulators and semiconductors
- Demand for the theoretical material design

Aim

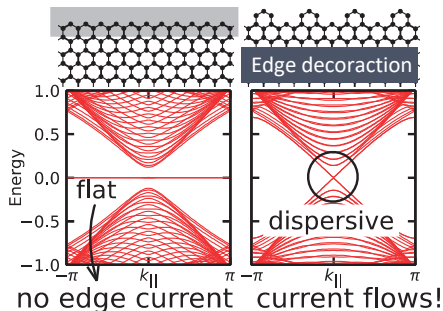
- Theoretical Proposal for controlling topologically protected surface/interface states
- Detailed analysis on the honeycomb lattice model as a prototype
- Investigation of electronic structures in a series of topological semimetals

Advanced Research Topics

Honeycomb lattice model

Honeycomb lattice + real space distortion

- Topologically nontrivial gap induced by an appropriate real space modulation
- Topological phase protected by the mirror symmetry



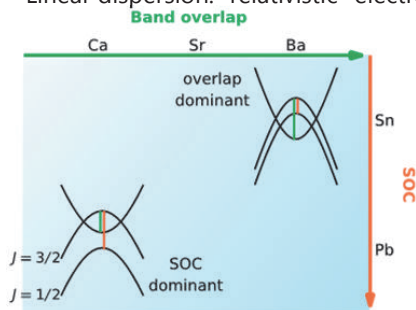
- Edge decoration dependence of the edge states

Topological Semimetals

Antiperovskite family A_3EO

$A=Ca, Sr, Ba / E=Sn, Pb$

- Topological semimetal with a linear dispersion near the Fermi energy
- Linear dispersion: "relativistic" electrons



- Control of relativistic electrons by competition between the spin-orbit coupling and band inversion

Publications

- T. Kariyado and X. Hu, *Sci. Rep.* **7**, 16515 (2017).
- T. Kariyado and M. Ogata, *Phys. Rev. Materials* **1**, 061201(R) (2017).

Summary

- Topological states and their edge shape dependence in a honeycomb lattice model
- Chemical composition dependence of the band structure of an antiperovskite family

Research outcome

- Potential switching devices making use of the edge shape dependence of the edge states
- Possible new functionalities by controlling relativistic electrons