Usage Report for Fiscal Year 2019

Project Title:

Materials properties under extreme conditions

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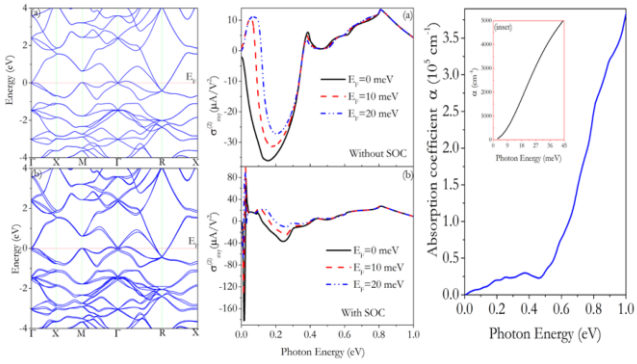
1. Background and purpose of the project, relationship of the project with other projects

Chiral topological semimetals have no spatial inversion symmetry and topologically non-trivial band structure. The nonlinear optical response of chiral topological semimetals has potential application for Terahertz generation and detection, because of the giant rectification current under Terahertz irradiation. However, the rectification current is dependent on some material parameters, such as spin-orbital coupling strength and the position of Fermi level. First-principles calculation is necessary for the optimal material candidate.

2. Specific usage status of the system and calculation method

First-principles calculation based on density functional theory, and Wannier function.

3. Result



The calculated band structure demonstrates triply degenerated band crossings at Γ and R point. The calculated second order optical conductivity is much larger when the spin-orbital coupling is included. Also, RiSh has very large absorption coefficient at Terahertz range.

4. Conclusion

Our calculation demonstrates that the maximal second order optical conductivity $\sigma^{(2)}_{zxy}$ (0; ω,−ω) of topological semimetal RhSi is about ~180 μA/V2 under an optical field with a photon energy of ~20 meV. With a photon energy large than 450 meV, $\sigma^{(2)}_{zxy}$ (0; ω,−ω) is relatively small. Especially, the calculated $\sigma^{(2)}_{zxy}$ (0; ω,−ω) is almost vanishing within a photon energy range of 450–500 meV. Below 300 meV, our calculation also reveals that the dielectric function and reflectivity decreases with an increase of photon energy, while the absorption coefficient increases with an increase of photon energy. Therefore, RhSi has a potential application for optoelectronic detection in the terahertz range.

5. Schedule and prospect for the future

There are two important topics in future. One is the material candidates for giant nonlinear optical response. The second is the Floquet topological matters.

6. If no job was executed, specify the reason.

Fiscal Year 2019 List of Publications Resulting from the Use of the supercomputer

- Zhi Li, Toshiaki Iitaka, Haibo Zeng, and Haibin Su, Optical response of the chiral topological semimetal RhSi, Phys. Rev. B 100, 155201 (2019).
- Zhi Li, Abudukadi Tudi, Peng Ren, Yun Yang, Toshiaki Iitaka, Takami Tohyama, Zhihua Yang, Shilie Pan, and Haibin Su, $NaPN_2$: Deep-ultraviolet nonlinear optical material with unprecedented strong second-harmonic generation coefficient, Phys. Rev. Materials 3, 025201 (2019).