Usage Report for Fiscal Year 2020

**Project Title:**

# Prediction of Crystal Structure and Properties

**Name:**

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

Nonlinear optical response of materials with broken spatial inversion symmetry has potential application for the generation and detection electromagnetic wave with specific frequency. Because of the giant rectification current of topological semimetals under Terahertz irradiation, the nonlinear optical effect of topological matters has attracted lots of research interest. However, the mechanism of rectification current in topological matter is still elusive. Also, the dependence between photocurrent and material parameters, such as spin-orbital coupling strength and the position of Fermi level, still need further research. First-principles calculation is necessary for the search of optimal material candidate.

2. Specific usage status of the system and calculation method

We perform the first-principles calculation based on density functional theory, and Wannier function on Hokusai system, including geometric optimization, electronic structure, and optical properties.

3. Result

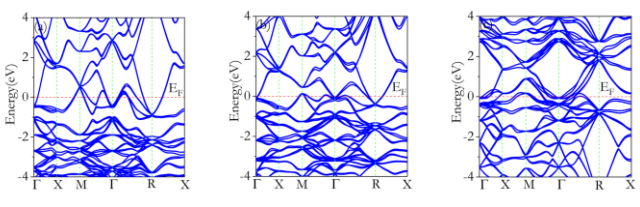


FIG. 1. Calculated band structure of (a) PdGa, (b) RhSn and (c) HfSn by the first-principles calculation with SOC.

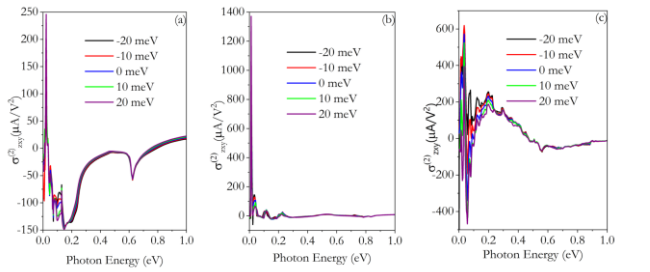


FIG. 2. Calculated shift vector mechanism contributed second-order optical conductivity of (a) PdGa, (b) RhSn and (c) HfSn by first-principles calculation with SOC.

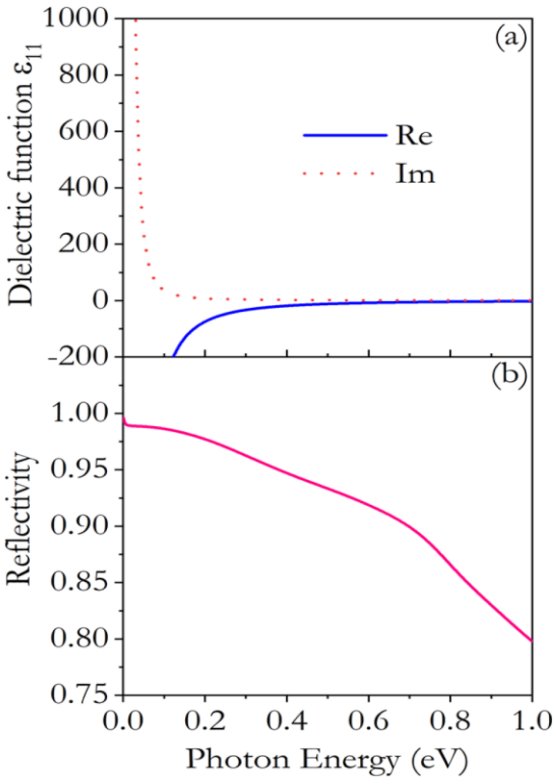


FIG. 3. (a) Calculated photon energy dependent dielectric function and (b) reflectivity of RhSn by first-principles calculation with SOC.

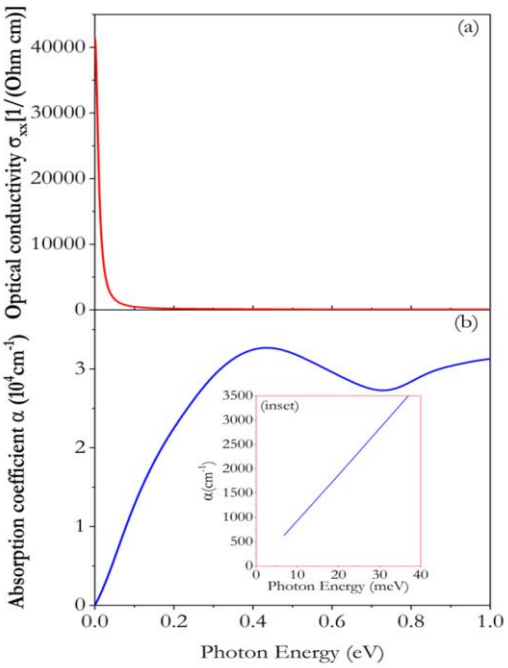


FIG. 4. Calculated photon energy dependent optical conductivity (a) and absorption coefficient (b) of RhSn by first-principles calculation with SOC.

4. Conclusion

Topological semimetals have linear band dispersion around the band crossing which is near the Fermi level. Chiral topological semimetals have no spatial inversion symmetry, and they have non-vanishing second order optical response. The band structure and nonlinear optical conductivity (NOC) σ_zxy^((2) ) (0;ω,-ω) of the isostructural chiral semimetals RhSn, HfSn, and PdGa are studied by the first-principles calculation in this work. Our calculation demonstrates that the maximal NOC σ_zxy^((2) ) (0;ω,-ω) of chiral semimetals RhSn is about ~1370 μA/V2 under terahertz optical field with photon energy of ~12 meV, while the maximal NOCs σ_zxy^((2) ) (0;ω,-ω) of HfSn and PdGa are 600 μA/V2 and 240 μA/V2, respectively. The relatively large NOC of RhSn can be interpreted by its multiple band crossing on the Fermi level, while multiple band crossings in the band structures of HfSn, and PdGa are not on the Fermi level. Our calculations also reveal that the calculated dielectric function decreases with increasing photon energy, while the absorption coefficient increases with increasing photon energy in the terahertz region. The relatively large NOC makes chiral topological semimetal RhSn suitable for terahertz detection.

5. Schedule and prospect for the future

There are two important topics in future. One is the material candidates for giant nonlinear optical response, including topological semimetals and heterojunction. The second is the intrinsic difference between CPGE and LPGE, and the effect of disorder, electronic correlation. Additionally, we will develop a python package to calculate the nonlinear optical response with different mechanisms.

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

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## Fiscal Year 2020 List of Publications Resulting from the Use of the supercomputer

### [Paper accepted by a journal]


1. Zhi Li, Yue Wang, Shengli Zhang, Toshiaki Iitaka, Takami Tohyama, Haibo Zeng, and Haibin Su, Optical-field induced SU(2) pair potential in caesium lead halide perovskites, International Journal of Modern Physics B Vol. 35, No. 2 (2021) 2150030 (10 pages)
2. Naotaka Tomioka, Luca Bindi, Takuo Okuchi, Masaaki Miyahara, Toshiaki Iitaka, Zhi Li, Tsutomu Kawatsu, Xiande Xie, Narangoo Purevjav, Riho Tani, and Yu Kodama, Poirierite, a dense metastable polymorph of magnesium iron silicate in shocked meteorites, *Commun Earth Environ* **2,** 16 (2021). https://doi.org/10.1038/s43247-020-00090-7