Usage Report for Fiscal Year 2021

Project Title:

Prediction of Crystal Structure and Properties

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

The linear electro-optic effect, is essentially a second order response under optical signal with high frequency and electric signal with low frequency. The general formalism for the second-order optical response of solids was proposed by Sipe and Shkrebtii. The lengthy formalism for electro-optic coefficient, which includes intra-band and inter-band contributions, applies to semiconductor under light field with relatively low photon energy. However, this requirement cannot be fulfilled in chiral topological semimetals. A new theory and computational method for electro-optic effect in topological semimetals should be developed. In the community of topological quantum matters, the low energy band dispersion near the Fermi level is classified by different fermions carrying Chern number. Especially, the linear band crossing plays the role of source or sink of Berry curvature. The new theory should also clarify that how does the Berry curvature or quantum geometric tensor affect the electro-optic effect. Since the Berry curvature in chiral topological semimetals is distributed in different energy scales, the chiral topological semimetals offer an excellent platform to investigate how the Berry curvature modifies the linear electro-optic effect and propagation of optical signal.

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 (including both linear and nonlinear response theory).

3. Result

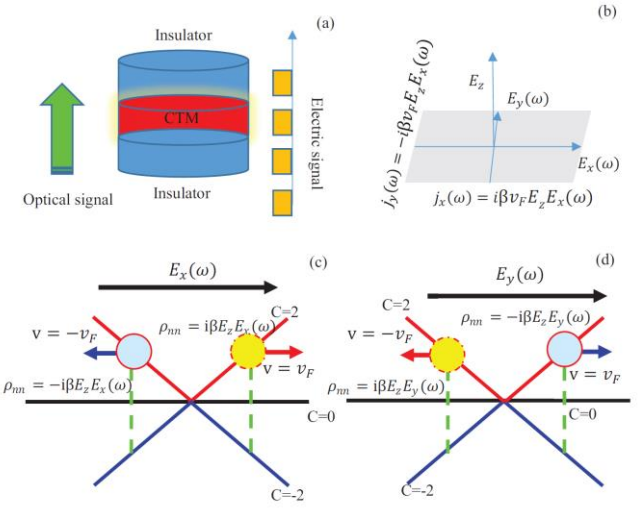

FIG. 1: (a) Schematic diagram for the electro-optic modulator consisting of chiral topological matter (CTM) and insulating cladding layers. (b) Nonlinear Hall current induced by Berry curvature, indicating the nonlinear Hall coefficient is antisymmetric. (c,d) Schematic diagrams for carrier generation and electronic velocity in momentum space, where β is a real coefficient. The chern number of each band is labelled by C.

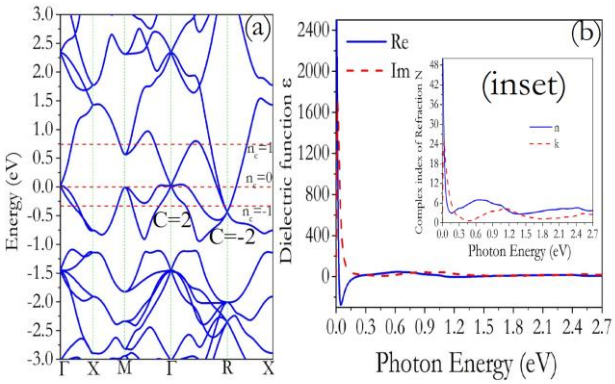

FIG. 2: The band structure of RhSi crystal without SOC, where the doping concentration n_c dependent Fermi level is marked by red dash line. Without doping, the Fermi level is set to 0 eV. The chiral fermions at Γ on Fermi level and the R point below Fermi level have opposite chirality. With electron (hole) doping concentration n_c=1 (n_c=-1), the Fermi level shifts to the higher (lower) red dash line. (b) Frequency dependent dielectric function $\epsilon(\omega)$ and complex refractive index $N = n(\omega) + ik(\omega)$ (inset) by the first-principles calculation within linear response. The peak at low frequency is dominated by intra-band contribution (Drude term).

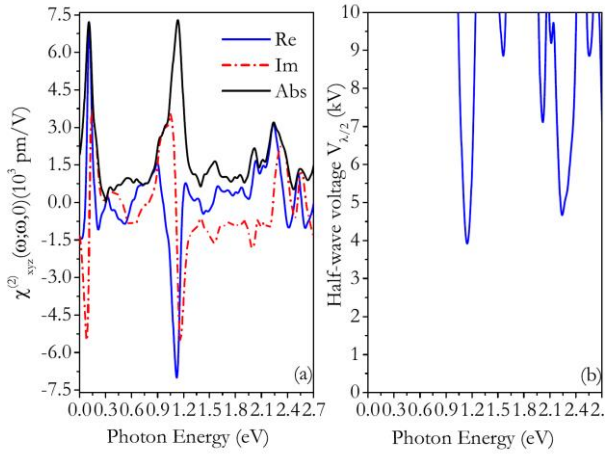

FIG. 3: (a) Frequency dependent electro-optic coefficient $\chi^{(2)}_{xyz}(\omega;\omega,0)$ contributed by shift current, where the real and imaginary parts are plotted by blue real line and red dash dot line, respectively. (b) Half-wave voltage determined by Eq. (11). At low frequency, the half-wave voltage is very high and out of range.

4. Conclusion

We identify that the linear electro-optic effect in chiral topological semimetals is dominated by oscillating nonlinear anomalous current and injection current, instead of shift current which dominates the linear electro-optic effect in semiconducting materials. The nonlinear optical conductivity σ(2) xyz(ω) contributed by the nonlinear anomalous current is antisymmetric under the exchange of indices x and y, and it is proportional to relaxation time and Chern number. With longer relaxation time or larger Chern number, the curvature involved currents can be significant enhanced, and renders a relatively low half-wave voltage for phase modulation. This work classifies that how does the Berry curvature modify the linear electro-optic effect in chiral topological semimetals and opens a new avenue to design the electro-optic modulator with half-wave voltage compatible with the CMOS circuit.

5. Schedule and prospect for the future

There are two important topics in future. One is developing efficient computational method for linear electro-optic coefficient for topological materials. Additionally, we will develop a python package to simulate the propagation of light in inhomogeneous medium.

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

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Fiscal Year 2021 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

1. Yuewen Gao, Toshiaki Iitaka, and Zhi Li, Terahertz nonlinear optics of chiral semimetals RhSn, HfSn, and PdGa, Eur. Phys. J. B (2021) 94:95
2. Zhi Li, Shengli Zhang, Takami Tohyama, Xiufeng Song, Yu Gu, Toshiaki Iitaka, Haibin Su, and Haibo Zeng, Optical detection of quantum geometric tensor in intrinsic semiconductors, Sci. China-Phys. Mech. Astron. 64, 107211 (2021).