Usage Report for Fiscal Year 2023

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 realization of fundamental particles in condensed matter has attracted lots of research interest, for example, massless Dirac fermions in graphene and Weyl fermions in TaAs. The massless Dirac fermion is characterized by a fourfold-degenerated band crossing, while the massless Weyl fermion is characterized by a twofold-degenerated band crossing. With broken time-reversal invariant symmetry or spatial inversion symmetry, the Dirac fermion can split into a pair of Weyl fermions with opposite chirality. Except for massless Dirac fermions and Weyl fermions, more unconventional quasiparticles beyond the standard model can be realized in condensed matter, provided the appropriate crystal symmetry is satisfied. For example, a threefold-degenerated band crossing has been proposed by calculation and verified by experiment in tungsten carbide and molybdenum phosphide. The band crossing in momentum space plays the role of the source of Berry curvature whose integral on a closed surface surrounding the band crossing defines the topological charge. The Weyl fermion in TaAs carries a topological charge of ±1, and the total topological charge is zero because of the no-go theorem. Chiral fermions with a higher topological charge are also proposed in numerous materials. Especially, the chiral transition metal silicides CoSi can host two types of unconventional fermions with topological charges of 2 and −2, respectively. Transition metal silicides CoSi, RhSi, RhGe, and CoGe crystallize into a simple cubic structure with the space group $P2_13$, which only includes rotational symmetry. Since there is no spatial inversion symmetry and mirror symmetry, the spin-1 fermion at the Γ point and charge-2 fermion at the R point are independent in the energy scale. In chiral crystals, the spatial inversion symmetry is broken, therefore second-order nonlinear effects including second harmonic generation (SHG) and the photocurrent effect are nonvanishing. Under circularly polarized light, the intraband photocurrent generation is referred to as a circular photogalvanic effect (CPGE), which is also dubbed the “injection current” and increases with time before a steady state is approached and the saturated current is only several nA/(W/cm^2), we will not emphasize the injection current in this work. Except for CPGE under circularly polarized light, there exists one more mechanism for the photocurrent, i.e., a shift vector induced photocurrent, which is nonvanishing under both linearly and circularly polarized light, provided the spatial inversion symmetry of the sample is broken. For most semiconductors, the photocurrent is dominated by an interband current induced by a shift vector which characterizes the difference in the Wannier center between the valence and conduction bands. However, there exists one more contribution to the photocurrent in chiral topological crystals, i.e., Berry curvature dipole induced photocurrent. This contribution is also proportional to the total topological charge of occupied states if circularly polarized light is applied. Under linearly polarized light, this contribution is completely vanishing. The total charge should be zero because of the time-reversal invariant symmetry in the chiral topological crystal. Therefore, the Berry curvature dipole induced photocurrent is also vanishing here. In this work, we calculated the photon energy dependent dielectric function, reflectivity, absorption coefficient, and second-order optical conductivity by first-principles calculation under high pressure. We predict that SiC can crystallize into *$P2_13$* under high pressure by the first-principles calculation. Further, we calculate the band structure and second-order optical conductivity of SiC with the space group *$P2_13$* to justify our proposal, via., high pressure is an efficiently approach to enhance the second-order optical conductivity.

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).

3. Result

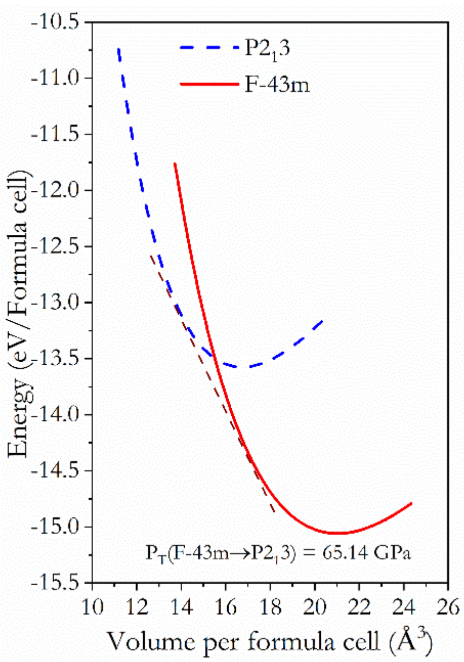

Fig. 1. The calculated EOS of SiC with the space group *F-43m* and *$P2_13$*. SiC will crystalize into a simple cubic structure will the space group *$P2_13$* under high pressure, and the phase transition pressure is 65.14 GPa.

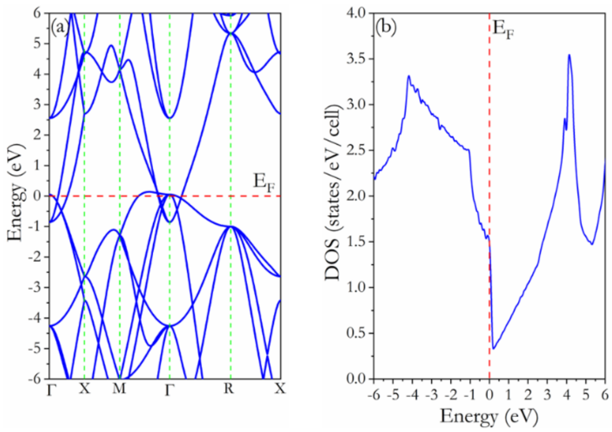

Fig. 2. Band structure (a) and DOS (b) of SiC with the space group *$P2_13$* by first-principles calculation.

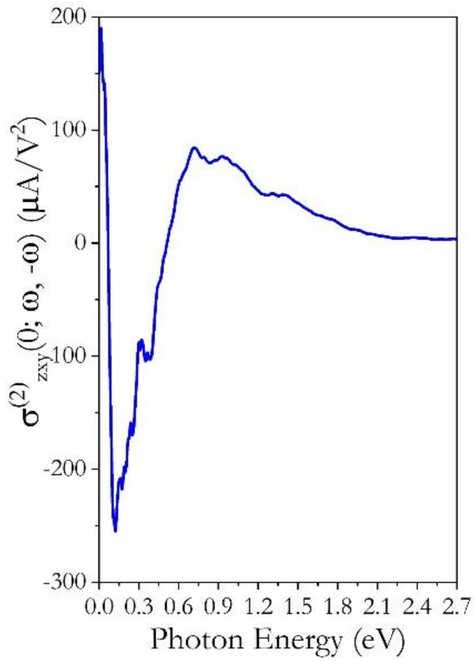

Fig. 3. Calculated shift vector mechanism contributed second-order optical conductivity of SiC with the space group *$P2_13$* by first-principles calculation.

4. Conclusion

In summary, we studied the electronic structure, dielectric function, reflectivity, and shift current of the chiral topological crystal SiC with the space group *$P2_13$* by first-principles calculation in the Wannier basis. Our calculation demonstrates that the second-order optical conductivity of SiC with the space group

$P2_13$ of is very large under an optical field with a photon energy smaller than 300 meV, and the maximal second-order optical conductivity is about ~250 μA/V^2 under an optical field with a photon energy of 150 meV, which is larger than that of RhSi. Additionally, our calculation also reveals that SiC with the space group *$P2_13$* has a relatively high absorption coefficient. Therefore, this work opens an avenue to design the potential application as photodetectors working in the terahertz range.

５. Schedule and prospect for the future

There is an important topic in future. We will explore better chiral topological crystals which can be a potential application as photodetectors working in the terahertz range.

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

Fiscal Year 2023 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Yuewen Gao, Yu Gu, Toshiaki Iitaka, and Zhi Li, Enhancement of the linear electro-optic effect by high pressure, PHYSICAL REVIEW B 107, 245203 (2023).