二次元 WTe_2 の非線形光学特性に関する計算

Simulation studies of nonlinear optical properties in two-dimensional Wely semimetal WTe_2

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研究成果概要

The Wely semimetal tungsten ditelluride (WTe_2) has attracted immense interest due to its fascinating physical properties and important applications as an example of topological quantum materials [1]. The novel phenomena of giant magneto-resistance are observed in Wely semimetal WTe_2 [2]. The electronic band structures of thin layered WTe_2 are determined by its layer number and stacking configuration including crystalline symmetry [3,4], which further influence the linear and nonlinear optical responses. In this study, we have simulated the linear and nonlinear optical responses of a few layer WTe_2 based on a real-time first principles approach including quasiparticle corrections. The electronic and optical properties in various structures of WTe_2 with different phases and stacking configurations were simulated by Quantum Espresso [5] and Yambo code [6]. The linear optical responses were calculated by Bethe-Salpeter equation (BSE)-GW methods and the nonlinear optical responses of second harmonic generation (SHG) were simulated by independent particle approximation (IPA) with quasi-particle corrections.

The monolayer 1T'- WTe_2 with $P2_1/m$ space group shows inactivity of SHG signals, while the monolayer Td- WTe_2 with Pm space group shows strong activity of SHG signals. The strong anisotropic second-order nonlinear susceptibility is observed due to low-symmetry crystal structures in monolayer Td- WTe_2. Moreover, the monolayer 2H- WTe_2 with P$\bar{6}$m2 space group shows activity of SHG signals, as similar to the other semiconducting MX_2 (M=Mo, W, X=S, Se). The results show that WTe_2 has unique phase-dependent optical properties including nonlinear optical responses, which are different from other two-dimensional transition metal dichalcogenides.

[1] S. Kimura, *et al. Phys. Rev. B* **99**, 195203 (2019).
[2] Y. Wang, *et al*. *Nano Lett.* **19**, 3969–3975 (2019).
[3] E. J. Sie, *et al. Nature* **565**, 61 (2019).
[4] J. Xiao *et al. Nat. Phys.* **16**, 1028 (2020).
[5] P. Giannozzi *et al., J. Phys.: Cond. Mat.* **29,** 465901 (2017).
[6] D. Sangalli *et al., J. Phys.: Cond. Mat.* **31,** 325902 (2019).