

二次元 WTe₂ 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 WTe₂

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研究成果概要

The Wely semimetal tungsten ditelluride (WTe₂) 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 WTe₂ [2]. The electronic band structures of thin layered WTe₂ 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 WTe₂ based on a real-time first principles approach including quasiparticle corrections. The electronic and optical properties in various structures of WTe₂ 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'-WTe₂ with P2₁/m space group shows inactivity of SHG signals, while the monolayer Td-WTe₂ 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-WTe₂. Moreover, the monolayer 2H-WTe₂ with P6m₂ space group shows activity of SHG signals, as similar to the other semiconducting MX₂ (M=Mo, W, X=S, Se). The results show that WTe₂ has unique phase-dependent optical properties including nonlinear optical responses, which are different from other two-dimensional transition metal dichalcogenides.

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