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原子層二次元半導体の励起子状態と光学特性の計算
Simulation of exciton states and optical properties in atomically thin semiconducting materials

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研究成果概要

The supercomputer system has been used for the *ab initio* simulation on the linear and nonlinear optical properties of thin layer SnS. Among the two-dimensional group IV monochalcogenides, tin monosulfide (SnS) has drawn much attention due to its superior optical and electronic properties. The monolayer SnS with the lack of inversion symmetry and in-plane anisotropy shows potential in the application of piezoelectric nanogenerators. The inversion symmetry and in-plane anisotropy has been evaluated by linear and nonlinear optical methods. However, the novel optical properties arising from inversion symmetry and in-plane anisotropy have not been fully understood in bilayer and thick layer SnS with various stacking structures. Herein, we intend to investigate the linear and nonlinear optical properties of SnS by *ab initio* simulation method.

Here, Quantum Espresso and Yambo code have been used in the supercomputer system for the *ab initio* simulation studies [1,2]. The bilayer SnS with four different stacking structures including AA stacking, AB stacking (α- and β$'$-type), and AC stacking are simulated. We have calculated the optical absorption spectra of bilayer SnS with consideration of many-body effect by solving Bethe-Salpeter equations. The absorption spectra clearly change according with the in-plane electric-field direction, which suggests the strong anisotropic wavefunction distribution of exciton states. The second harmony generation (SHG) susceptibility is also calculated under various field directions. We have also simulated the polar-pattern of SHG intensity in AB stacking bilayer SnS in the parallel and perpendicular detected configuration. The strong and anisotropic SHG intensity also implies the anisotropic piezoelectricity. These results could provide useful information towards the application of SnS in piezoelectric devices.

[1] P. Giannozzi *et al., J. Phys.: Cond. Mat.* **29,** 465901 (2017).
[2] D. Sangalli *et al., J. Phys.: Cond. Mat.* **31,** 325902 (2019).