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| **第 1 条，共 1 条** |
| **标题:** FIRST-PRINCIPLES CALCULATION OF THERMAL AND OPTICAL PROPERTIES OF MOLYBDENUM DISULFIDE |
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| **摘要:** The thermal and optical properties of layered structures of molybdenum disulfide (MoS2) were studied based on the first-principles density functional theory. The phonon density of states in various layered and bulk MoS2 shows a discontinuous band gap between about 7.0 and 8.0 THz. The specific heat variation with temperature and other thermodynamic properties like the Helmholtz free energy, entropy, and total energy are similar between the layered structures and bulk MoS2. The specific heat increases rapidly with increasing temperature in the region < 500 K and nearly flattens when the temperature goes above 1000 K. For the temperature < 400 K, the electronic plus vibrational Helmholtz free energy is positive, indicating electrons can be easily restricted to the MoS2 layers. The layered structures affect the optical properties in both in-plane and through-plane substantially. The monolayer has the lowest values of the dielectric function, optical conductivity, and absorptive index, whereas the bulk material shows the highest ones correspondingly. For the real refractive index, the monolayer has the lowest value at the low energy level, but could go to the highest in the interval from 15.0 eV to 35.5 eV or exceeding 37.6 eV. The band gap of the layered structures generally decreases with increasing layer number. The calculated band gap for the MoS2 bilayer at 1.78 eV matches with the experimental measurement in the literature. |
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