DFT and DFPT calculations of 3R and 2H polytypes of Molybdenum Disulfide

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The structural, optoelectronic, vibrational, including infrared and Raman theoretical spectra, and thermodynamic properties of 3R- and 2H- polytypes of molybdenum disulfide (MoS$_2$) are studied using Density Functional Theory (DFT) considering both the local density and generalized gradient approximation, LDA and GGA, respectively. Calculated lattice parameters are close to the experimental measurements, and an indirect band gap $E(\Gamma \rightarrow \Lambda) = 1.33 \text{ eV}$ (0.68 eV) was obtained within the GGA (LDA) level of calculation, considering the 3R- polytype, and for the 2H- polytype an indirect band gap $E(\Gamma \rightarrow \Lambda) = 1.30 \text{ eV}$ (0.70 eV) was obtained within the GGA (LDA) approximation. The complex dielectric function and absorption of 3R-MoS$_2$ and 2H-MoS$_2$ polytypes were shown to be sensitive to the plane of polarization of the incident light. The phonon dispersion relation together with density of states (DOS) as well as theoretical peaks of the infrared (IR) and Raman spectra in the frequency range of 0-800 cm$^{-1}$ was analyzed and assigned, considering the norm-conserved pseudopotentials. The thermodynamic potentials, the specific heat at constant volume and Debye temperature of the 3R-MoS$_2$ and 2H-MoS$_2$ polytypes are also calculated, whose dependence with the temperature are discussed. The structure 2H-MoS$_2$ crystal become a little more stable energetically than 3R-MoS$_2$ crystal as the temperature increases, and for physical applications that require thermal insulation, would be more appropriate to use the 3R-MoS$_2$ phase.

Reference: