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Dimensionality-dependent Electronic and Optical Properties of MoS_2 GEORGIOS KOPIDAKIS, DAPHNE DAVELOU, ARISTEA E. MANIADAKI, GEORGE KIOSEOGLOU, IOANNIS N. REMEDIAKIS, Dept of Materials Science and Technology, University of Crete — We present theoretical calculations based on Density-Functional Theory (DFT) for MoS_2, a layered material which can be shaped into single-layer and several other nanostructures with unique catalytic, mechanical, electronic and optical properties. We consider ribbons, single-layer, bilayer and bulk structures, at equilibrium and under hydrostatic strain. We calculate the electronic band structure and use linear-response theory to obtain the imaginary part of the dielectric function. Other optical properties, such as absorption and reflectivity, are also calculated. Strain changes dramatically the electronic structure, as it induces changes in the location of both the conduction band minimum and the valence band maximum. Single layer MoS2 becomes an indirect-gap semiconductor while a direct gap is observed at zero strain. The results of the simulations are in good agreement with experimental measurements of energy-dependent reflectivity and photoluminescence spectra. We compare the dielectric properties of bulk (3D), single-layer (2D) and ribbons (1D) of MoS2 and discuss general trends of the macroscopic dielectric constant as a function of dimensionality. Some closely related dichalcogenides will also be discussed.

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