

Abstract Submitted
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Two-Dimensional Semiconductors From Theory to Experiments: MoS₂ and MoSe₂ CAN ATACA, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States, SEFAATTIN TONGAY, J. ZHOU, K. LO, JUNQIAO WU, Department of Material Science and Engineering, University of California, Berkeley, Berkeley, California 94720, United States — After the synthesis of graphene, single layer transition metal dichalcogenides have been shown to possess superior optical properties than those of graphene. Until now, both theorists and experimentalists have mainly focused on the properties of single-layer MoS₂. In this work, the first synthesis of single and few layers of MoSe₂ are shown experimentally and are complemented by stability analysis through phonon and electronic structure calculations using density functional theory (DFT). The DFT calculations include van der Waals and spin-orbit interactions which are shown to play an important role in the geometric structure, electronic, magnetic and vibrational properties. Single-layer MoSe₂ is measured and calculated as a direct band gap material, having band gap values suitable for solar cells and optical devices. Dimensionality effects predicted by DFT calculations such as variation of the energy band structures and Raman active vibrational modes are confirmed by experiments. Optical and electronic properties of single and few layers MoSe₂ can be tuned by varying the temperature, number of layers and applying pressure to the samples. Single layer MoS₂ and MoSe₂ possess a number of properties that make them highly promising materials for future nanoscale applications.

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