Electronic and optical properties of monolayer and few-layer films of InSe and GaSe

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Abstract

We present the analysis of electronic band structure of InSe and GaSe films, from the stoichiometric mono- to N-layer films, and we describe the resulting optical properties of these 2D materials [1,2] and conduction/valence band parameters. This study is based on the ab initio DFT and related multi-orbital tight-binding model analysis of the electronic band structure and wave functions in the two-dimensional N-layer InSe crystals, and it is compared to the results of luminescence spectroscopy of this material. We show [1-3] that the band gap in InSe (and GaSe) strongly depend on the number of layers, with a strong (more than twice) reduction from the monolayer to crystals with N>6. We find that the conduction-band-edge electron mass in few-layer InSe is quite light (comparable to Si), which suggests opportunities for high-mobility devices and the development of nanocircuits. In contrast, the valence band in mono-, bi- and trilayer InSe is flat, opening