Abstract

The discovery of graphene stimulated significant interest towards two dimensional materials owing to their unique structural, electronic, magnetic and other properties. Semiconducting transition metal dichalcogenides (TMDs) represent a class of layered materials with nonzero band gap, and as a result attract great attention.

Density functional theory (DFT) is a method of choice for theoretical exploration of condensed matter. However, there exists well-known problem with band gap evaluation within DFT framework. Significant efforts were made to solve DFT band gap problem, still the results may vary significantly. Relatively accurate results for band gaps could be obtained by GW approximation. However, sometimes GW fails for more than 30% in band gap value and it is computationally expensive method. Thus, general theoretical approach for accurate band gap computation within DFT is in big demand, which can be used for exploration of new materials with the required properties.

We recently proposed new general approach (GVJ-2e-method) for band gap calculation within DFT framework, which is based solely on total energies calculation and is adjustable parameter free. The GVJ-2e method was verified on wide range of materials from bulk semiconductors (ex. Si, C, Ge) to wide gap insulators (ex. Xe, Kr) and yielded band gap results with practically experimental accuracy. The errors of proposed method are smaller than errors of other widely used methods (GW, hybrid functional HSE, TB-mBJ functional).

The thesis presents the results of applying the proposed method for the study of the properties of TMDs. First, the structural stability of bulk and monolayer TMDs (MoS_2, $MoSe_2$, WS_2, WSe_2) have been studied. For $MoS_{2(1-x)}Se_{2x}$ alloy structural stability with increasing concentration of Se have been analyzed also at microscopic level (different relative positions of Se atoms in alloy). The electronic properties (band gaps and density of states) of bulk and monolayer TMDs, and $MoS_{2(1-x)}Se_{2x}$ alloy are obtained. The calculated with GVJ-2e method band gaps are used in interpretation of experimental results for bulk and monolayer TMDs, and $MoS_{2(1-x)}Se_{2x}$ alloy.