Electronic Properties of Bulk and Monolayer TMDs: Theoretical Study Within DFT Framework (GVJ-2e Method)

Julia Gusakova (Foreign) [1],

Xingli Wang (Foreign) [2],

Li Lynn Shiau (Foreign) [3],

Anna Krivosheeva [4],

Victor Shaposhnikov [5],

Victor Borisenko [6],

Vasilii Gusakov (Foreign) [7],

Beng Kang Tay (Foreign) [8]

2017

1, 2, 3, 7, 8 Foreign

4, 5, 6 Belarusian State University of Informatics and Radioelectronics P. Browka 6, 220013 Minsk, Belarus

Keywords: Band gap, density functional theory, electronic properties, layered materials, TMD.

Abstract: Accurate prediction of band gap for new emerging materials is highly desirable for the exploration of potential applications. The band gaps of bulk and monolayer TMDs (MoS2, MoSe2, WS2, and WSe2) are calculated with the recently proposed by us GVJ-2e method, which is

implemented within DFT framework without adjustable parameters and is based on the total energies only. The calculated band gaps are in very good agreement with experimental ones for both bulk and monolayer TMDs. For monolayer MoS2, MoSe2, WS2, and WSe2, direct band gaps are predicted to be 1.88 eV, 1.57 eV, 2.03 eV, 1.67 eV correspondingly, and for bulk TMDs, indirect band gaps of 1.23 eV (MoS2), 1.09 eV (MoSe2), 1.32 eV (WS2), 1.21 eV (WSe2) are predicted. The GVJ-2e method demonstrates good accuracy with mean absolute error (MAE) of about 0.03 eV for TMDs PL gaps (and 0.06 eV for QP gaps). GVJ-2e method allows to equally accurately obtain band gaps for 3D and 2D materials. The errors of GVJ-2e method are significantly smaller than errors of other widely used methods such as GW (MAE 0.23 eV), hybrid functional HSE (MAE 0.17 eV), TB-mBJ functional (MAE 0.14 eV).

Published in:

Electronic properties of bulk and monolayer TMDs: theoretical study within DFT framework GVJ-2e method, Phys. Status Solidi A 214(12), 1700218 (7 pages) (2017). – DOI: 10.1002/pssa.201700218.

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