Band gap calculation of bulk and monolayer transition metal dichalcogenides with new GVJ-2E approach within DFT framework

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**Abstract/Аннотация:** We have calculated fundamental band gaps for bulk and monolayer transition metal dichalcogenides (TMDs: MoS2, MoSe2, WS2, and WSe2) with recently proposed by us GVJ-2e method. The calculated band gaps are in a good agreement with experimental ones for both bulk and monolayer TMDs, having mean absolute error (MAE) of about 0.03 eV. The errors of GVJ-2e method are significantly smaller than those of other widely used ones such as GW (MAE 0.35 eV) and hybrid functional HSE (MAE 0.17 eV).

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