Electronic band structures of molybdenum and tungsten dichalcogenides by the *GW* approach

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Supporting Information

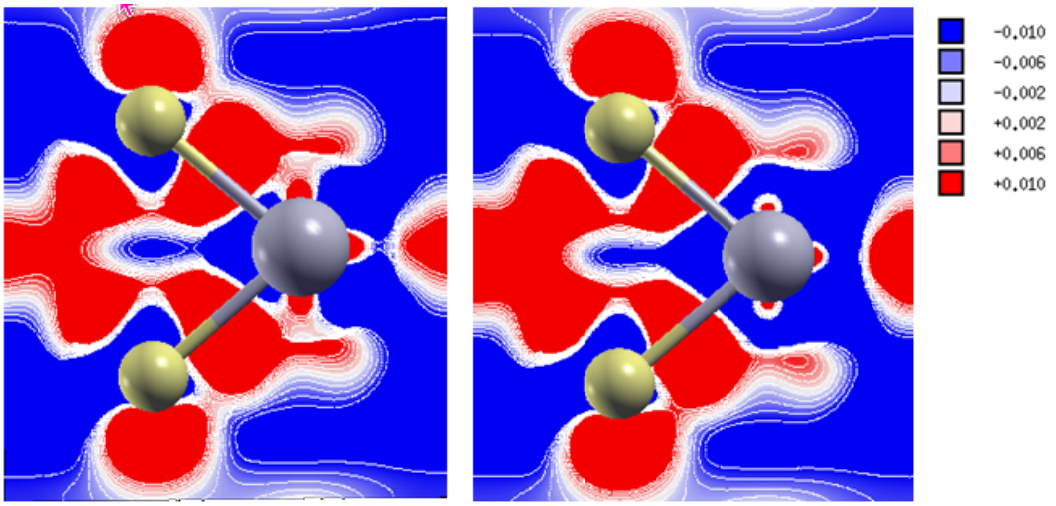

Figure S1: The 2D contour plot of electron density difference, i.e. the difference between the electron density of MX_2 and the overlap of free-atom density, in MoS_2 (Left) and WS_2 (right). The big balls represent Mo or W atoms, and the small balls represent S atoms. Overall there is a strong depletion (accumulation) of electrons around M (X) atoms, and the charge transfer is more significant in WS_2 than in MoS_2. Bader's atom-in-molecule analysis indicates that in MoS_2, Mo and S atoms have effective charges of 1.22 and -0.61, respectively, while in WS_2, W and S have effective charges of 1.37 and -0.68, implying that the chemical bonding in WS_2 is more ionic than MoS_2.

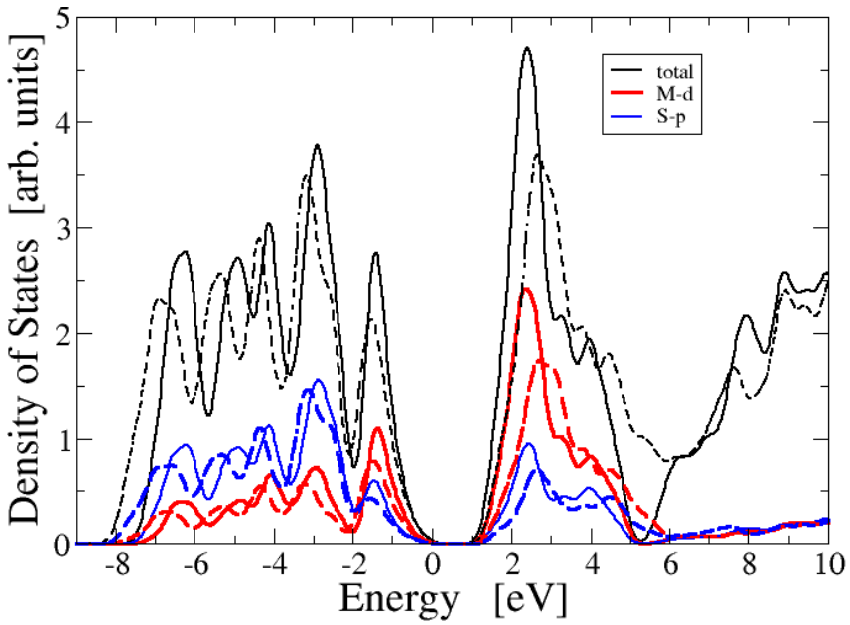

Figure S2: Comparison of the density of states of MoS_2 (solid) and WS_2 (dashed) from the GW calculations.

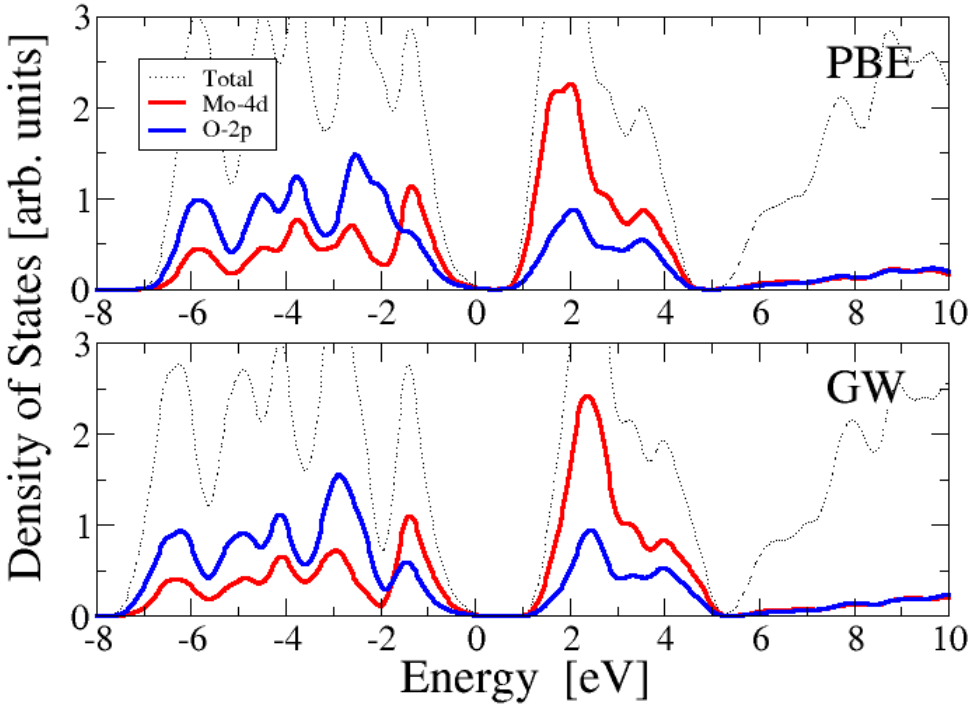

Figure S3: Comparison of projected density of states (PDOS) of MoS_2 obtained from PBE and GW calculations. Note that GW PDOS is calculated by using the GW quasi-particle energies but with PBE wave-functions.