Erratum: "Quasiparticle electronic structure of phthalocyanine:TMD interfaces from first-principles GW" [J. Chem. Phys. 155, 214702 (2021)]

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In a subsequent investigation, we have found an error in our previously reported[1] GW electronic structure of the H_2Pc:MoS_2 interface when the composite system is supported on a SiO_2 substrate.

The correct line in Table I should be:

TABLE I. Key descriptors of the electronic structure for the H_2Pc:MoS_2 interface adsorbed on SiO_2 using GW. All values are in eV. Δ^0_{TMD} and Δ^0_{mol} are the band gaps of the freestanding TMD monolayer and molecular layer, respectively. Δ^0_{TMD} is calculated at the K point for the unit cell, and Δ^0_{mol} is calculated at the Γ point. Δ_{TMD}, Δ_{LL}, Δ_{HL}, Δ_{HH}, and Δ_{mol} are energy level differences within the interface systems defined in Fig. 2 of the original paper, all calculated at the Γ point.

	Interface	Method	Type	Δ^0_{TMD}	Δ_{TMD}	Δ_{LL}	Δ_{HL}	Δ_{HH}	Δ_{mol}	Δ^0_{mol}
Originally reported in Ref. 1	H_2Pc:MoS_2:SiO_2	GW	IIa, Fig. 2(c)	2.81	2.07	0.68	1.62	0.45	2.30	3.86
Corrected result	H_2Pc:MoS_2:SiO_2	GW	IIa, Fig. 2(c)	2.81	2.70	0.13	2.25	0.45	2.38	3.86

Correspondingly, the correct Fig. 4 of the paper should be:

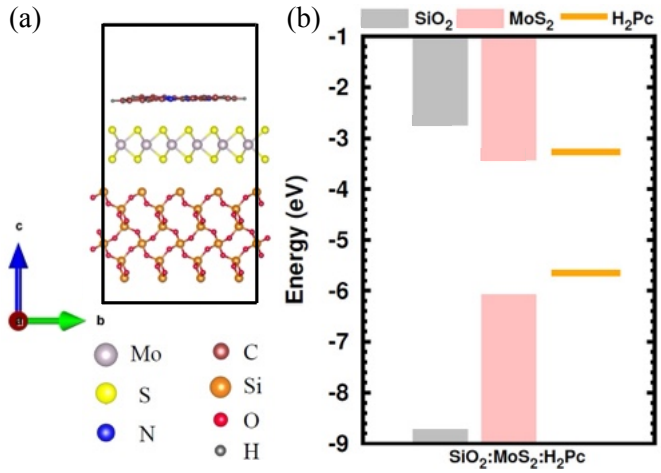

FIG. 4. (a) (This panel stays the same as in Ref. 1) Optimized structure of the H_2Pc:MoS_2:SiO_2 interface. (b) (This panel is corrected in this erratum) Quasiparticle energy level alignment from an embedding GW calculation, where the H_2Pc:MoS_2 interface is embedded into a dielectric environment of a SiO_2 substrate. All energy levels are measured with respect to vacuum.

Consequently, the substrate effect of SiO_2 is not as strong as we originally determined. Compared to the H_2Pc:MoS_2 interface, the SiO_2 substrate has a moderate effect of renormalizing the MoS_2 gap by about 0.08 eV. Due to the dielectric screening of SiO_2, the gap of H_2Pc within the H_2Pc:MoS_2 interface is renormalized by 0.09 eV, and the gap of the H_2Pc:MoS_2 interface is renormalized by 0.08 eV. The Δ_{LL} and Δ_{HH} in the H_2Pc:MoS_2 interface are nearly not affected by the SiO_2 substrate. This moderate screening effect of the SiO_2 substrate is consistent with Refs. 2–4, where the change in the band gap of MoS_2 is found to be in the 0.09-0.25 eV range when monolayer MoS_2 (without an H_2Pc molecule) is deposited on SiO_2 substrate.

This erratum does not alter the results of all other calculations without the SiO_2 substrate or the structure-property relationship that we predicted using GW in Ref. 1.

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