Erratum: Interactions between copper and transition metal dichalcogenides: A density functional theory study [Phys. Rev. Materials 1, 034001 (2017)]

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In the original article, the density functional theory (DFT) calculations of the conduction-band minimum (CBM) and the valence-band maximum (VBM) for VX_2 only took one of the electron spins into account. If both spins are taken into account, the band alignment is modified slightly, affecting the Schottky barrier calculations. Hence, our statements that VS_2 and VSe_2 would form Schottky barriers with Cu(111) is incorrect. Interestingly, the corrected results better fit the overall trend that we see regarding Schottky barriers: The transition metal dichalcogenides (TMDs) of groups IV and V do not appear to form Schottky barriers with Cu(111), but the TMDs of group VI appear to form Schottky barriers roughly 0.5 eV in height. Figures E1 and E2 are corrected versions of Figs. 10 and 11 in the original paper, and the corrected data are highlighted. Furthermore, the units of the charge density in Fig. 8(d) should also be listed as electrons/Å, instead of eV/Å, and the energy difference between the T and T' phases of VTe_2 should be listed as 17 meV instead of 36 meV.

We also discovered typographical and spreadsheet errors in some of the tables included in the Supplemental Material [1]. The corrected data are provided in Tables E1–E4 with corrected values highlighted in red. Corrections to the cohesive energies result in root-mean-square percent errors of approximately 10% for the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE) and approximately 12% for GGA-PBE with the DFT-D3 van der Waals correction against the available experimental data. The changes are minor and do not affect our results or conclusions.

The k -grid sizes listed in the *Assessment of Calculation Accuracy* section of the Supplemental Material [1] should be listed as $18 \times 18 \times 4$ and $18 \times 18 \times 8$ for the 2H and 1T phases, respectively. However, the k -grids for the GGA-PBE calculations were $18 \times 18 \times 4$ for both the 2H and the 1T phases.

Finally, the atomic structures in Figs. 6, 8(c), and S2 in the Supplemental Material [1] were rendered using VESTA [2]. A citation to the program should be given, and is provided in the bibliography of this paper.

The PYTHON programming language [3,4], including the NUMPY [5,6], SCIPY [7], and ATOMIC SIMULATION ENVIRONMENT [8] packages, in addition to the VTST tools of the Henkelman Research Group [9], were used in the postprocessing of the DFT data; plots were created using MATPLOTLIB [10] or the ORIGINPRO software maintained by the OriginLab Corporation.

FIG. E1. Correction to Fig. 10 where the labels of the modified data are colored green: Representation of Schottky barrier formation in the Cu/TMD hybrids as a result of the potential step: the Schottky barrier in the semiconductor TMDs is the vertical offset ϕ from the lower line, which has slope 1. Note that χ_{TMD} for the metallic TMDs is simply the Fermi level. Open symbols indicate DFT + U results. The phase of each TMD is that corresponding to the favored freestanding structure as shown in Fig. 7.

FIG. E2. Correction to Fig. 11 where the modified data are circled: Band alignment for (a) freestanding TMDs in the ground-state phase and (b) the hybrid Cu(111)/TMD slabs with the Fermi energy of a pure copper slab $E_{F,Cu}$, long horizontal black line for comparison. The Fermi level E_F , CBM, and VBM are given for each freestanding and hybrid structure as the short black, red, and blue horizontal lines. Half-length lines indicate the Fermi level, CBM, and VBM obtained from DFT + U for VX_2 . The phase of the TMD is indicated by H or T.

TABLE E1. Correction to Table S2 with changes in red: Lattice matching parameters (n_1, n_2, m_1, m_2), supercell size, number of TMD formula units (F), total number of atoms in the supercell (N), supercell parameter (a), and the strain on the Cu slab for the two lowest-strain orientations of the 15 H phase TMDs. Negative strains indicate compression of the Cu slab; positive strains indicate tension.

TMD	Lowest strain orientation						Second lowest strain orientation					
	n_1, n_2, m_1, m_2	TMD supercell Cu supercell	F	N	a (Å)	Cu strain (%)	n_1, n_2, m_1, m_2	TMD supercell Cu supercell	F	N	a (Å)	Cu strain (%)
MoS ₂	2, 2, 2, 3	$\sqrt{12} \times \sqrt{12}$ $\sqrt{19} \times \sqrt{19}$	12	150	10.96	-0.32	0, 4, 5, 0	4×4 5×5	16	198	12.65	+0.35
MoSe ₂	1, 2, 2, 2	$\sqrt{7} \times \sqrt{7}$ $\sqrt{12} \times \sqrt{12}$	7	93	8.72	-0.17	2, 0, 1, 2	2×2 $\sqrt{7} \times \sqrt{7}$	4	54	6.59	-1.20
MoTe ₂	3, 1, 0, 5	$\sqrt{13} \times \sqrt{13}$ 5×5	13	189	12.69	+0.67	1, 2, 3, 1	$\sqrt{7} \times \sqrt{7}$ $\sqrt{13} \times \sqrt{13}$	7	99	9.31	+2.44
WS ₂	2, 2, 2, 3	$\sqrt{12} \times \sqrt{12}$ $\sqrt{19} \times \sqrt{19}$	12	150	10.98	-0.13	0, 4, 5, 0	4×4 5×5	16	198	12.68	+0.54
WSe ₂	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$ $\sqrt{12} \times \sqrt{12}$	7	93	8.70	-0.38	2, 0, 1, 2	2×2 $\sqrt{7} \times \sqrt{7}$	4	54	6.58	-1.40
WTe ₂	1, 3, 0, 5	$\sqrt{13} \times \sqrt{13}$ 5×5	13	189	12.68	+0.56	1, 2, 3, 1	$\sqrt{7} \times \sqrt{7}$ $\sqrt{13} \times \sqrt{13}$	7	99	9.30	+2.33
NbS ₂	0, 2, 2, 1	2×2 $\sqrt{7} \times \sqrt{7}$	4	54	6.68	+0.11	3, 0, 4, 0	3×3 4×4	9	123	10.02	-0.68
NbSe ₂	1, 2, 1, 3	$\sqrt{7} \times \sqrt{7}$ $\sqrt{13} \times \sqrt{13}$	7	99	9.16	+0.74	1, 3, 5, 0	$\sqrt{13} \times \sqrt{13}$ 5×5	13	189	12.48	-1.00
NbTe ₂	2, 2, 0, 5	$\sqrt{12} \times \sqrt{12}$ 5×5	12	186	12.64	+0.28	3, 0, 2, 3	$\sqrt{19} \times \sqrt{19}$ $\sqrt{19} \times \sqrt{19}$	9	141	10.95	-0.38
TiS ₂	0, 2, 1, 2	2×2 $\sqrt{7} \times \sqrt{7}$	4	54	6.66	-0.13	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$ $\sqrt{12} \times \sqrt{12}$	7	93	8.81	+0.91
TiSe ₂	1, 3, 0, 5	$\sqrt{13} \times \sqrt{13}$ 5×5	13	189	12.55	-0.45	1, 2, 3, 1	$\sqrt{7} \times \sqrt{7}$ $\sqrt{13} \times \sqrt{13}$	7	99	9.21	+1.30
TiTe ₂	0, 3, 3, 2	3×3 $\sqrt{19} \times \sqrt{19}$	9	141	11.16	+1.52	2, 0, 3, 0	2×2 3×3	4	66	7.44	-1.66
VS ₂	2, 2, 2, 3	$\sqrt{12} \times \sqrt{12}$ $\sqrt{19} \times \sqrt{19}$	12	150	10.97	-0.19	0, 4, 5, 0	4×4 5×5	16	198	12.67	+0.47
VSe ₂	0, 2, 1, 2	2×2 $\sqrt{7} \times \sqrt{7}$	4	54	6.65	-0.34	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$ $\sqrt{12} \times \sqrt{12}$	7	93	8.80	+0.69
VTe ₂	1, 3, 0, 5	$\sqrt{13} \times \sqrt{13}$ 5×5	13	189	12.84	+1.80	2, 2, 5, 0	$\sqrt{12} \times \sqrt{12}$ 5×5	12	186	12.33	-2.19

TABLE E2. Correction to Table S3 with changes in red: Lattice matching parameters (n_1, n_2, m_1, m_2), supercell size, number of TMD formula units (F), total number of atoms in the supercell (N), supercell parameter (a), and strain on the Cu slab for the two lowest-strain orientations of the 15 T phase TMDs. Negative strains indicate compression of the Cu slab; positive strains indicate tension.

TMD	Lowest strain orientation						Second lowest strain orientation					
	n_1, n_2, m_1, m_2	TMD supercell Cu supercell	F	N	a (Å)	Cu strain (%)	n_1, n_2, m_1, m_2	TMD supercell Cu supercell	F	N	a (Å)	Cu strain (%)
MoS ₂	0, 4, 0, 5	4 × 4	16	198	12.59	−0.11	2, 2, 3, 2	$\sqrt{12} \times \sqrt{12}$	12	150	10.91	−0.77
		5 × 5						$\sqrt{19} \times \sqrt{19}$				
MoSe ₂	1, 3, 4, 1	$\sqrt{13} \times \sqrt{13}$	13	165	11.72	+1.43	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$	7	93	8.6	−1.54
		$\sqrt{21} \times \sqrt{21}$						$\sqrt{12} \times \sqrt{12}$				
MoTe ₂	1, 2, 1, 3	$\sqrt{7} \times \sqrt{7}$	7	99	9.15	+0.62	1, 3, 5, 0	$\sqrt{13} \times \sqrt{13}$	13	189	12.47	−1.12
		$\sqrt{13} \times \sqrt{13}$						5 × 5				
WS ₂	2, 2, 3, 2	$\sqrt{12} \times \sqrt{12}$	12	150	11.01	+0.20	3, 1, 4, 1	$\sqrt{13} \times \sqrt{13}$	13	165	11.46	−0.80
		$\sqrt{19} \times \sqrt{19}$						$\sqrt{21} \times \sqrt{21}$				
WSe ₂	1, 3, 4, 1	$\sqrt{13} \times \sqrt{13}$	13	165	11.70	+1.28	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$	7	93	8.59	−1.69
		$\sqrt{21} \times \sqrt{21}$						$\sqrt{12} \times \sqrt{12}$				
WTe ₂	1, 2, 1, 3	$\sqrt{7} \times \sqrt{7}$	7	99	9.15	+0.65	1, 3, 5, 0	$\sqrt{13} \times \sqrt{13}$	13	189	12.47	−1.09
		$\sqrt{13} \times \sqrt{13}$						5 × 5				
NbS ₂	0, 3, 0, 4	3 × 3	9	123	10.09	<+0.01	0, 2, 1, 2	2 × 2	4	54	6.73	+0.80
		4 × 4						$\sqrt{7} \times \sqrt{7}$				
NbSe ₂	1, 2, 1, 3	$\sqrt{7} \times \sqrt{7}$	7	99	9.16	+0.79	1, 3, 5, 0	$\sqrt{13} \times \sqrt{13}$	13	189	12.49	−0.95
		$\sqrt{13} \times \sqrt{13}$						5 × 5				
NbTe ₂	2, 2, 0, 5	$\sqrt{12} \times \sqrt{12}$	12	186	12.55	−0.43	3, 0, 2, 3	3 × 3	9	141	10.87	−1.09
		5 × 5						$\sqrt{19} \times \sqrt{19}$				
TiS ₂	0, 3, 0, 4	3 × 3	9	123	10.19	+1.05	2, 1, 3, 1	$\sqrt{7} \times \sqrt{7}$	7	99	8.99	−1.13
		4 × 4						$\sqrt{13} \times \sqrt{13}$				
TiSe ₂	1, 3, 0, 5	$\sqrt{13} \times \sqrt{13}$	13	189	12.70	+0.73	1, 2, 3, 1	$\sqrt{7} \times \sqrt{7}$	7	99	9.32	+2.50
		5 × 5						$\sqrt{13} \times \sqrt{13}$				
TiTe ₂	0, 2, 0, 3	2 × 2	4	66	7.46	−1.41	3, 0, 3, 2	3 × 3	9	141	11.19	+1.79
		3 × 3						$\sqrt{19} \times \sqrt{19}$				
VS ₂	2, 2, 2, 3	$\sqrt{12} \times \sqrt{12}$	12	150	10.98	−0.13	0, 4, 5, 0	4 × 4	16	198	12.68	+0.54
		$\sqrt{19} \times \sqrt{19}$						5 × 5				
VSe ₂	0, 2, 1, 2	2 × 2	4	54	6.64	−0.44	2, 1, 2, 2	$\sqrt{7} \times \sqrt{7}$	7	93	8.79	+0.59
								$\sqrt{12} \times \sqrt{12}$				
VTe ₂	1, 3, 0, 5	$\sqrt{13} \times \sqrt{13}$	13	189	12.75	+1.15	2, 2, 5, 0	$\sqrt{12} \times \sqrt{12}$	12	186	12.25	−2.82
		5 × 5						5 × 5				

TABLE E3. Correction to Table S5 with changes in red: Bulk TMD cohesive energies per formula unit compared to the experimental enthalpy of formation.

TMD	Bulk cohesive energy (eV/MX ₂)			% Difference		
	DFT-D3	GGA-PBE	Expt.	DFT-D3	GGA-PBE	Expt. Ref.
2H-MoS ₂	-2.64	-2.66	-2.80	-5.64	-4.91	[11]
2H-MoSe ₂	-2.03	-2.05	-2.40	-15.39	-14.73	[12], [13]
2H-MoTe ₂	-0.70	-0.80				
2H-WS ₂	-2.30	-2.45	-2.50	-8.03	-2.11	[14]
2H-WSe ₂	-1.62	-1.65	-1.90	-14.53	-12.97	[11]
2H-WTe ₂	-0.05	-0.18				
2H-NbS ₂	-3.06	-3.07				
2H-NbSe ₂	-2.56	-2.56				
2H-NbTe ₂	-1.26	-1.34				
2H-TiS ₂	-3.34	-3.41				
2H-TiSe ₂	-2.92	-2.99				
2H-TiTe ₂	-1.64	-1.81				
2H-VS ₂	-2.47	-2.61				
2H-VS ₂ ^a	-2.54	-2.68				
2H-VSe ₂	-1.96	-2.12				
2H-VSe ₂ ^a	-2.06	-2.22				
2H-VTe ₂	-0.76	-0.84				
2H-VTe ₂ ^a	-0.86	-1.00				
1T-MoS ₂	-1.83	-1.82				
1T-MoSe ₂	-1.35	-1.34				
1T-MoTe ₂	-0.18	-0.28				
1T-WS ₂	-1.42	-1.56				
1T-WSe ₂	-0.87	-0.88				
1T-WTe ₂	0.52	0.39				
1T-NbS ₂	-2.95	-2.96				
1T-NbSe ₂	-1.43	-2.46				
1T-NbTe ₂	-1.19	-1.28				
1T-TiS ₂	-3.76	-3.84				
1T-TiSe ₂	-3.27	-3.35				
1T-TiTe ₂	-1.92	-2.09				
1T-VS ₂	-2.44	-2.57				
1T-VS ₂ ^a	-2.49	-2.62				
1T-VSe ₂	-1.94	-2.09				
1T-VSe ₂ ^a	-2.04	-2.19				
1T-VTe ₂	-0.79	-0.92				
1T-VTe ₂ ^a	-0.94	-1.08				

^aIncludes the Hubbard U parameter for $V3d$ orbitals: $U = 2.00$ eV and $J = 0.87$ eV ($U_{\text{eff}} = 1.13$ eV).

TABLE E4. Correction to Table S6 with changes in red: Comparison of binding energy (E_b), equilibrium separation distance (d , between Cu surface and bottom chalcogen atoms in the first TMD layer), Schottky barrier (ϕ), and potential step (ΔV) for monolayer and bilayer H-MoSe₂ and H-NbS₂ adsorbed on Cu(111).

	MoSe ₂				NbS ₂			
	d (Å)	E_b (J/m ²)	ΔV (eV)	ϕ (eV)	d (Å)	E_b (J/m ²)	ΔV (eV)	ϕ (eV)
Monolayer	2.39	1.50	0.52	0.52	2.05	2.33	-0.99	
Bilayer	2.39	1.54	0.46	0.45	2.06	2.39	-1.19	

- [1] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevMaterials.1.034001> for a comparison of bulk TMD lattice parameters with experiment, tabulated Cu/TMD interface orientations and strain, and a brief examination of Cu(111) interfaces with multilayer TMDs.
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