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Addition/Correction

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Correction to "Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach"

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The estimation of the correction to the calculated hydrogen adsorption energy to obtain the free energy of adsorption is wrong. We state in the present version of the manuscript (pg 1578 column 2) that the zero-point correction for the adsorbed hydrogen is 0.39 eV and that for the H_2 molecule is 0.54 eV. The correct values should be 0.20 and 0.27 eV. This means that the correction to the energy becomes 0.26 eV instead of the quoted 0.32 eV. The conclusions of the Letter are essentially unchanged because the error is smaller than the calculated error bars on the individual calculated heats of formation and much smaller than the energy window of 0.5 eV used for identifying good HER candidates. Furthermore, the estimated correction is just an estimate based on a single system (MoS_2) and can be expected to have some variation from system to system that is not taken into account. However, because of the change in the correction term Figure 6 and the last column of Table 3 change in detail. The changes are fairly small, but because the probability factor P is used for ordering, some of the systems are swapped in Figure 6 and Table 3. We have included the figure and table the way they would look if a correction value of 0.26 eV is used instead.

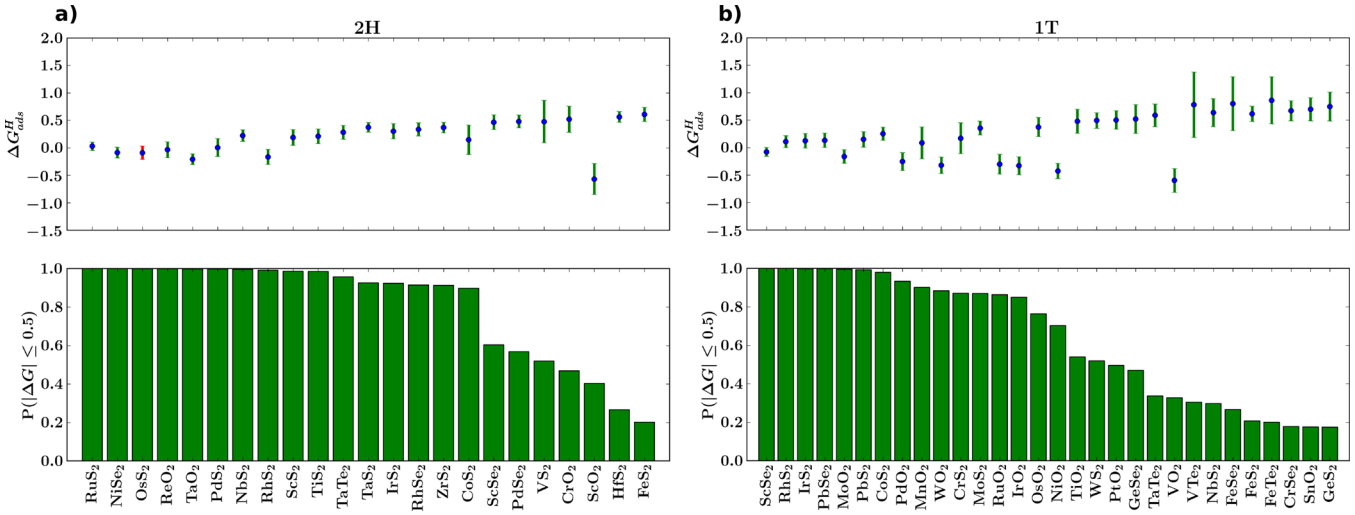

Figure 6.

Table 3

2 H-MX_2	ΔH	ΔH_{hull}[a]	δH_{hull}	$\Delta H_{expt.}$	ref 1	$\Delta H_{2H/1T}$	$P(\lvert\Delta G\rvert \leq 0.5)$
RuS_2	−0.31	−0.70	0.39	−0.71	no	−0.01	1.00
$NiSe_2$	−0.21	−0.34	0.13	−0.38	no	0.17	1.00
OsS_2	0.34	−0.60	0.94	NA	no	−0.01	1.00
ReO_2	−0.91	−1.42	0.51	−1.52	no	0.05	1.00
TaO_2	−2.58	−3.00	0.42	NA	no	−0.07	1.00
PdS_2	0.01	−0.31	0.32	−0.28	yes	0.17	1.00
NbS_2	−1.21	−1.20	−0.01	NA	yes	−0.04	1.00
RhS_2	−0.11	−0.48	0.37	NA	no	0.07	0.99
ScS_2	−1.46	−1.46	0.00	NA	no	−0.06	0.99
TiS_2	−1.23	−1.37	0.14	−1.41	yes	0.15	0.98
$TaTe_2$	−0.32	−0.45	0.13	NA	yes	0.00	0.96
TaS_2	−1.24	−1.22	−0.02	−1.22	yes	−0.02	0.93
IrS_2	−0.11	−0.48	0.37	−0.46	no	0.22	0.92
$RhSe_2$	−0.17	−0.45	0.28	NA	no	0.07	0.92
ZrS_2	−1.55	−1.73	0.18	−1.99	yes	0.19	0.91

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Table 3 Continued

2 H-MX_2	ΔH	ΔH_{hull}[a]	δH_{hull}	$\Delta H_{expt.}$	ref 1	$\Delta H_{2H/1T}$	$P(\lvert\Delta G\rvert \leq 0.5)$
CoS_2	−0.33	−0.48	0.15	−0.51	no	0.01	0.90
$ScSe_2$	−1.30	−1.25*	−0.05	NA	no	−0.01	0.60
$PdSe_2$	−0.02	−0.33	0.31	NA	yes	0.22	0.57
VS_2	−1.16	−1.14	−0.02	NA	no	−0.02	0.52
CrO_2	−1.99	−2.15	0.16	−2.01	no	0.03	0.47
ScO_2	−2.74	−3.17*	0.43	NA	no	0.05	0.40
HfS_2	−1.62	−1.80	0.18	NA	yes	0.22	0.26
FeS_2	−0.54	−0.73	0.19	−0.59	no	0.05	0.06
1 T-MX_2	ΔH	ΔH_{hull}[a]	δH_{hull}	$\Delta H_{expt.}$	ref 1	$\Delta H_{1T/2H}$	$P(\lvert\Delta G\rvert \leq 0.5)$
$ScSe_2$	−1.34	−1.25*	−0.09	NA	no	0.01	1.00
RhS_2	−0.32	−0.48	0.16	NA	no	−0.07	1.00
IrS_2	−0.30	−0.48	0.18	−0.46	no	−0.22	1.00
$PbSe_2$	0.04	−0.31*	0.35	NA	no	−0.22	1.00
MoO_2	−1.79	−1.95	0.16	−2.04	no	0.31	1.00
PbS_2	0.03	−0.32*	0.35	NA	no	−0.28	0.99
CoS_2	−0.34	−0.48	0.14	−0.51	no	−0.01	0.98
PdO_2	−0.48	−0.41	−0.07	NA	no	NA	0.93
MnO_2	−2.00	−1.98	−0.02	−1.80	no	−0.43	0.90
WO_2	−1.61	−1.89	0.28	NA	no	0.24	0.88
CrS_2	−0.77	−0.71	−0.06	NA	yes	0.12	0.87
MoS_2	−0.66	−0.93	0.27	−0.95	yes	0.28	0.87
RuO_2	−0.71	−0.94	0.23	−1.05	no	−0.20	0.86
IrO_2	−0.70	−0.94	0.24	−0.86	no	NA	0.85
OsO_2	−0.23	−1.10	0.87	−1.02	no	NA	0.76
NiO_2	−1.01	−0.79*	−0.22	NA	no	NA	0.70
TiO_2	−3.10	−3.29	0.19	−3.26	no	−1.11	0.54
WS_2	−0.59	−0.78	0.19	−0.90	yes	0.18	0.52
PtO_2	−0.61	−0.62	0.01	NA	no	NA	0.50
$GeSe_2$	−0.27	−0.34	0.07	−0.39	no	NA	0.47
$TaTe_2$	−0.32	−0.45	0.13	NA	yes	0.00	0.34
VO_2	−2.47	−2.63	0.16	−2.48	no	−0.10	0.32
VTe_2	−0.40	−0.45	0.05	NA	yes	0.00	0.30
NbS_2	−1.18	−1.20	0.02	NA	yes	0.04	0.30
$FeSe_2$	−0.48	−0.56	0.08	NA	no	−0.05	0.26
FeS_2	−0.61	−0.73	0.12	−0.59	no	−0.06	0.21
$FeTe_2$	−0.11	−0.20	0.09	−0.25	no	−0.02	0.20
$CrSe_2$	−0.63	−0.46	0.17	NA	yes	0.02	0.18
SnO_2	−1.33	−2.10	0.77	−1.99	no	NA	0.18
GeS_2	−0.42	−0.55	0.13	−0.42	no	NA	0.17

[a]The symbol * in superscript corresponds to the situation where no bulk structure with the compound composition lies on the convex hull according to the database. In that case, ΔH_{hull} is calculated as a linear combination of several structures.

REFERENCES

(1) Lebègue, S.; Björkman, T.; Klintenberg, M.; Nieminen, R. M.; Eriksson, O. Two-Dimensional Materials from Data Filtering and *Ab Initio* Calculations. *Phys. Rev. X* **2013**, *3*, 031002.

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