Supplementary Material

Accurate Formation Enthalpies of Solids Using Reaction Networks

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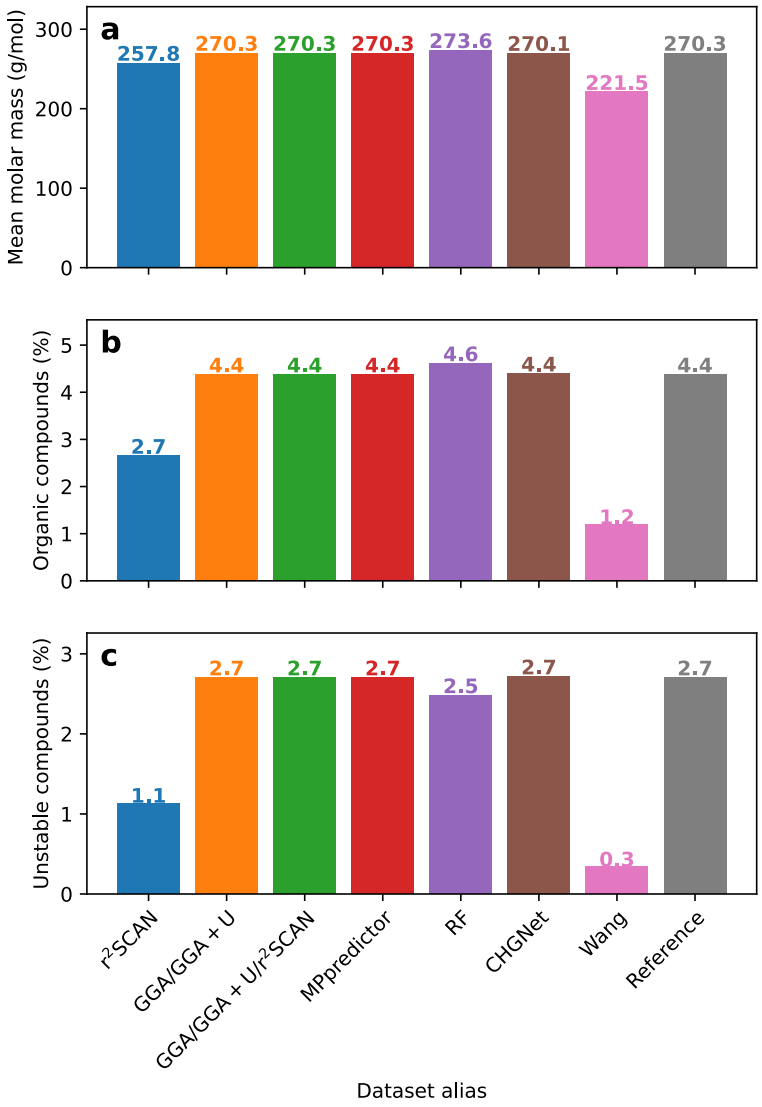
1 Datasets

1.1 Statistics



Supplementary Figure 1: Various statistics of the datasets considered in the paper (see Table 1, for further information about the individual datasets). For a compound in a given dataset, the compound is considered unstable if $\Delta_{\mathrm{f}} H_{\mathrm{ref}} > 0$ (ref is Reference) for this compound.

1.2 Data-validation

Supplementary Table 1: Significant disagreements, between experimental values of $\Delta_f H$ from the NBS reference dataset ($\Delta_f H_{ref}$) and from values in the Wang data-set [1]. All values are reported in eV atom^{-1}. These compounds are not included in the main data-sets.

`likely_mpid`	Formula	Reference	Wang
mp-1018028	TiS	-1.233	-1.410
mp-12765	GdC_2	-0.363	-0.257
mp-1336	PdO	-0.443	-0.599
mp-1479	BP	-0.409	-0.599
mp-18511	NdF_3	-4.293	-4.438
mp-19760	$Na_2Mo_2O_7$	-2.115	-2.225
mp-1984	TaS_2	-1.603	-1.223
mp-2071	Zn_3P_2	-0.980	-0.330
mp-21075	HfC	-1.303	-1.171
mp-21856	Co_2SiO_4	-2.187	-2.071
mp-22205	InN	-0.091	-0.716
mp-22216	In_2S_3	-0.885	-0.737
mp-22856	Bi_2S_3	-0.297	-0.418
mp-22870	InBr	-0.908	-0.106
mp-23162	$ZrCl_2$	-1.734	-1.489
mp-27719	$CuAl_2O_4$	-2.684	-2.883
mp-2815	MoS_2	-0.812	-0.954
mp-29555	$MoBr_2$	-0.902	-0.701
mp-438	Nd_2S_3	-2.463	-2.333
mp-540828	FeOCl	-1.302	-1.411
mp-542613	GeS_2	-0.655	-0.542
mp-684638	Al_2S_3	-1.501	-1.349
mp-700	GeSe	-0.477	-0.358
mp-9813	WS_2	-0.722	-0.896

Supplementary Table 2: Significant disagreements between experimental values of $\Delta_f H$ from the NBS reference dataset ($\Delta_f H_{ref}$) and from various literature sources ($\Delta_f H_{lit}$). $\Delta_f H_{lit}$ is reported as a single value or a range of values. In some cases no value is reported but estimate(s) of a closely related property, related compound or supporting calculations suggest that there is significant uncertainty/inaccuracy in $\Delta_f H$ for the compound in question. All values are reported in eV atom^{-1}. These compounds are not included in the main datasets.

`likely_mpid`	Formula	Reference	Literature	Literature source
mp-1188188	Mn_3C	0.012	-0.103	[2]
mp-1274	CoS	-0.429	–§	[3]
mp-1347	Th_3P_4	-1.691	–§	[4]
mp-13862	$B_{13}P_2$	-0.115	–§	[4]
mp-1415	CaSe	-1.908	-2.145	[5]
mp-1550	AlP	-0.863	-0.671†	[4]
mp-1598	Na_3P	-0.240	-0.523 to -0.257‡	[4]
mp-15668	Na_2Se_2	-0.970	–§	[5]
mp-2011	UP	-1.389	-1.689†	[4]
mp-22488	Co_2C	0.145	0.010	[6]
mp-2296	Ni_3P	-0.544	-0.919 to -0.309†	[4]
mp-23162	$ZrCl_2$	-1.734	-1.834	[7]
mp-24290	S_7NH	-0.325	0.103	[8]
mp-2441	Cd_3P_2	-0.238	–§	[4]
mp-2490	GaP	-0.912	–§	[4]
mp-2662	MnP	-0.586	-0.713†	[4]
mp-2758	SrSe	-1.999	-2.104	[5]
mp-27440	ZrCl	-1.368	-1.555	[7]
mp-29014	P_2S_3	-0.167	-0.324	[9]
mp-413	UP_2	-1.054	–§	[4]
mp-560553	IrF_6	-0.858	-1.316	[10]
mp-560613	Na_2TeO_4	-1.660	-1.445	[11]
mp-561511	FeAsS	-0.145	–§	[12]
mp-568264	$SiSe_2$	-0.100	-0.613	[5]
mp-739	TiP	-1.466	–§	[4]
mp-7463	Cu_3P	-0.393	-0.396 to -0.176†	[4]
mp-787	U_3P_4	-1.239	-1.840†	[4]
mp-927	CuP_2	-0.418	-0.498 to -0.260†	[4]
mp-931	ThP	-1.804	–§	[4]
mp-972	MnSe	-0.553	-0.922	[5]

† The reference state that has been for P used in the source (red V) has been converted to the reference state used in the reference data (α-white), using the suggested enthalpy difference in [4].

‡ Unknown which reference state(s) are used for P.

§ No value is reported in the source, but estimate(s) of a closely related property, related compound or supporting calculations suggest that there is significant uncertainty/inaccuracy in $\Delta_f H$ for this compound.

Compounds for which $\Delta_f H_{ref}$ is considered unreliable with reference to the literature values of Wang et al. are given in Table 1. Compounds for which $\Delta_f H_{ref}$ is considered unreliable with reference to miscellaneous literature values are given in Table 2. If the same compound was found in both cases, the entry belonging to Table 2 is reported. $\Delta_f H_{ref}$ is considered unreliable if it differs from the literature values $\Delta_f H_{lit}$ by ≥ 0.1 eV atom^{-1} or if no explicit value is provided for $\Delta_f H_{ref}$ but there is reason to believe that the reference value is highly uncertain.

Supplementary Table 3: Mismatches between Materials Project's (MP) composition/formula and the matched ICSD entry. These compounds are not included in the main data-sets.

`likely_mpid`	Formula (MP)	Formula (ICSD)	ICSD identifier
mp-1057216	LiS	LiSH	25590
mp-1180691	KVO_4	$KVO_3 \cdot H_2O$	24728
mp-1193254	$Sr(CO_2)_2$	$Sr(HCO_2)_2$	151246
mp-1197831	$LiBrO_3$	$LiBrO_2 \cdot H_2O$	4323
mp-1204504	$U(CO_3)_2$	$(UO_2)_2(OH)_2(C_4O_4)(H_2O)_2$	248209
mp-643934	$CuH_2(CO_2)_2$	$Cu(HCOO)_2 \cdot 4\,H_2O$	109965
mp-727410	K_2SnCl_4O	$K_2SnCl_4 \cdot H_2O$	76169
mp-726693	$TlCl_3$	$TCl_3 \cdot 4\,H_2O$	20760

Supplementary Table 4: Compounds for which a more likely materials project id was found (likely_mpid) during the data processing, after initial assignments (assigned mpid) had been made. These compounds are not included in the main datasets.

assigned mpid	`likely_mpid`	Formula	Reference
mp-1017565	mp-612740	In_2Se_3	[5]
mp-10264	mp-203	NiTe	[13]
mp-1045	mp-2763	Nd_2O_3	[14]
mp-1078295	mp-3671	$NaNbO_3$	[15]
mp-1195863	mp-1192688	$Zn(N_3)_2$	[16]
mp-15651	mp-662	NiSe	[5]
mp-16705	mp-2063	Pr_2O_3	[14]
mp-19443	mp-619461	WO_3	[17]
mp-20530	mp-780712	$CeCrO_3$	[18]
mp-218	mp-1745	Sm_2O_3	[14]
mp-2292	mp-1968	La_2O_3	[14]
mp-24834	mp-23790	NH_4NO_3	[19]
mp-294	mp-1198490	UO_3	[14]
mp-504886	mp-643084	Gd_2O_3	[14]
mp-505531	mp-2099	FeS	[20]
mp-551905	mp-540783	OsO_4	[21]
mp-552185	mp-669466	$AgNO_3$	[22]
mp-554278	mp-2657	TiO_2	[9]
mp-571453	mp-23499	K_2SnCl_6	[23]
mp-571486	mp-488	CuSe	[5]
mp-583213	mp-23192	HgI_2	[24]
mp-696658	mp-557263	$CH_3NH_3NO_3$	[25]
mp-707535	mp-1181584	$CH_4N_4O_2$	[26]
mp-9813	mp-224	WS_2	[27]

Supplementary Table 5: Compounds for which the crystal structure was found to be discrepant or unclear with respect to the NBS reference data (see Comment column), after initial assignments (assigned mpid) had been made. These compounds are not included in the main datasets.

assigned mpid	Formula	Comment	Reference
mp-1077078	KCN	wrong polymorph	[28]
mp-1106356	AlH_3	wrong polymorph	[9]
mp-1179716	$RbHCO_3$	wrong compound	[29]
mp-1195133	$Ca(CH_2OHCO_2)_2$	wrong compound	[30]
mp-1393	$AuSn_4$	wrong symmetry	[31]
mp-18905	FeO	uncertain structure	[32]
mp-1984	TaS_2	uncertain polymorph	[33]
mp-29687	KC_{60}	uncertain polymorph	[34]
mp-30053	NaCN	wrong polymorph	[28]
mp-32539	WO_2Cl_2	uncertain structure	[35]
mp-554867	Ta_2O_5	wrong polymorph	[36]
mp-560282	$K_2Ba(NO_2)_4$	wrong polymorph	[37]
mp-567366	$CsCuCl_3$	wrong polymorph	[38]
mp-570634	Cd_3As_2	wrong polymorph	[39]
mp-643099	$CNH(NH_2)_2 \cdot HNO_3$	wrong polymorph	[40]
mp-680506	$PtCl_4$	uncertain structure	[41]
mp-721084	$NH_4I \cdot NH_3$	wrong polymorph	[42]

Supplementary Table 6: Compounds with $\Delta_{\text{hull}}H_{\text{MP}} > 0.2$ eV atom^{-1}, $|\Delta_{\text{hull}}H_{\text{MP}}$-$\Delta_{\text{f}}H_{\text{MP}}| > 0.2$ eV atom^{-1} and not satisfying $0.85\text{V}_{\text{ICSD}} < \text{V}_{\text{MP}} < 1.1\text{V}_{\text{ICSD}}$. $\Delta_{\text{hull}}H_{\text{MP}}$, $\Delta_{\text{f}}H_{\text{MP}}$, V_{MP} are the default Materials Project GGA/GGA+U/r^{2}SCAN values for the energy above hull, formation enthalpy and unit cell volume, respectively. V_{ICSD} is the experimental volume and $\Delta_{\%}\text{V}$ is the percentage difference between V_{MP} and V_{ICSD}. Enthalpies/Energies are in eV atom^{-1} and volumes are in Å^3/atom.

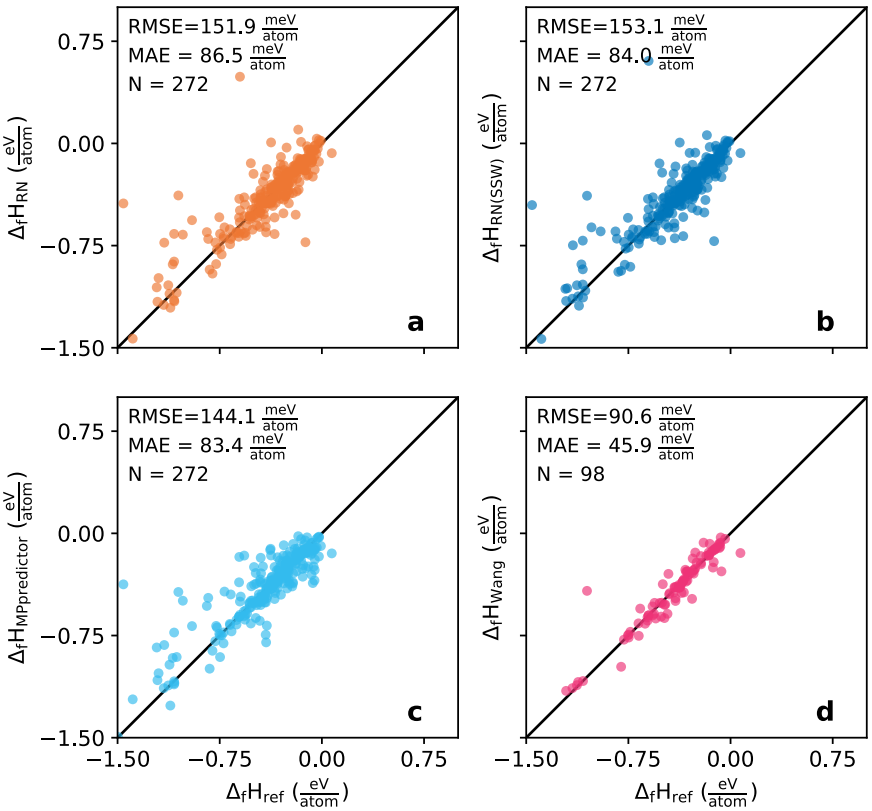
likely_mpid	Formula	$\Delta_{\text{hull}}H_{\text{MP}}$	$\Delta_{\text{f}}H_{\text{MP}}$	V_{MP}	V_{ICSD}	$\Delta_{\%}\text{V}$	ICSD ID
mp-13862	$B_{13}P_2$	0.96	0.65	10.8	8.15	32.0	23923
mp-5282	$Ag_2C_2O_4$	0.22	-1.10	14.0	12.4	12.9	109601
mp-560574	$Hg(CN)_2 \cdot HgO$	0.49	0.11	20.6	18.7	10.4	25708
mp-642662	$SrCl_2 \cdot H_2O$	0.29	-1.80	19.0	16.7	13.8	60883
mp-653562	$Ag_3I(NO_3)_2$	0.23	-0.41	17.2	15.4	11.8	14248
mp-696849	$NaBO_2 \cdot 4\,H_2O$	0.33	-1.29	11.1	9.4	18.0	34652
mp-699496	$K_2Cd(SO_4)_2 \cdot 2\,CdSO_4 \cdot 5\,H_2O$	0.46	-1.24	13.2	11.6	14.0	96214
mp-707471	$ZnI_2 \cdot 4\,NH_3$	0.59	0.06	15.6	13.4	16.2	78972
mp-707786	$Ba(OH)_2 \cdot 8\,H_2O$	0.61	-0.81	11.4	8.6	32.2	33741
mp-721035	$Cu(NH_3)_4(NO_3)_2$	0.88	-0.04	11.9	8.9	33.9	369
mp-721144	$Na_4P_2O_7 \cdot 10\,H_2O$	0.37	-1.31	5.7	4.7	19.5	15389
mp-836079	$Mn_2(CO)_{10}$	0.61	-0.79	8.8	7.8	13.4	415718

Supplementary Table 7: Compounds for which no prediction could be made.

likely_mpid	Formula
mp-1201095	$H_4Fe(CN)_6$
mp-1427	Lu_2O_3
mp-24445	$Nd_2(SO_4)_3 \cdot 8\,H_2O$
mp-571448	Cs_2PuCl_6
mp-642318	$(Ba(NO_2)_2)_2 \cdot TlNO_2$

Table 7 lists the compounds for which no reactions could be found. For Lu_2O_3, $Nd_2(SO_4)_3 \cdot 8\,H_2O$ and Cs_2PuCl_6, the exclusion of compound-sets through data-validation removed all possible reactions. For $H_4Fe(CN)_6$ and $(Ba(NO_2)_2)_2 \cdot TlNO_2$ no reactions were found at all with the current settings.

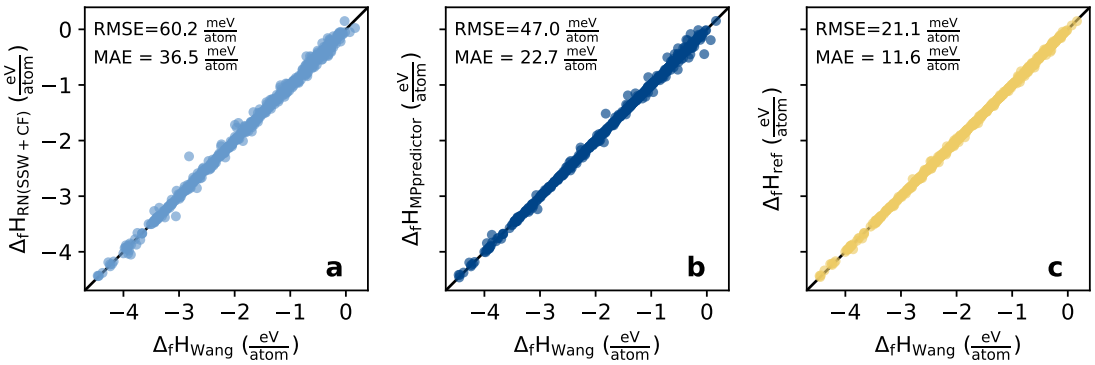
1.3 The intermetallic compounds



Supplementary Figure 2: Formation enthalpies predicted using several methods compared to the experimental reference data for the intermetallic compounds: (**A**) r^{2}SCAN(GGA/GGA+U)-RN predictions. (**B**) r^{2}SCAN(GGA/GGA+U)-RN(SSW) predictions. (**C**) MPpredictor predictions. (**D**) Wang experimental data. RMSE is the root mean squared error, MAE is the mean absolute error and N is the number of compounds considered.

We define an intermetallic compound as a solid phase containing two or more metallic elements. Metalloids are included in the definition of metallic elements. For predictions of the intermetallics all intermetallics were included in the reaction space. Figure 2 shows some analysis of the intermetallic compounds in the context of other methods/data-sets. Only the SSW variant is shown because the chemistry-guided filter has not been optimized to account for intermetallic chemistry.

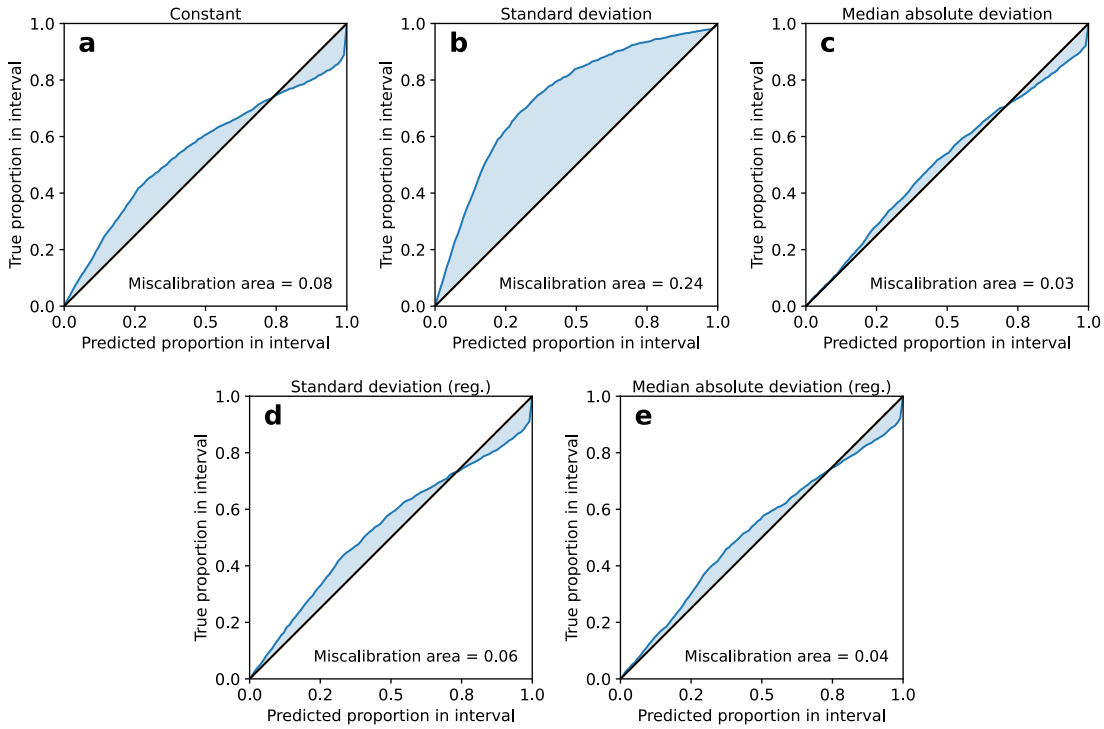
2 Comparison with Wang et al. experimental data



Supplementary Figure 3: Formation enthalpies predicted using several methods compared to experimental data from Wang [1] for 586 compounds part of the Table 1 data-sets: (**A**) r^{2}SCAN(GGA/GGA+U)-RN(SSW+CF) predictions. (**B**) MPpredictor predictions. (**C**) Reference data. RMSE is the root mean squared error, MAE is the mean absolute error. Note that outliers have been removed (Table 1 and Table 2 and this data does not contain the intermetallics).

In Figure 3 the Wang experimental dataset[1] is considered against other data. MPpredictor performs better than r^{2}SCAN(GGA/GGA+U)-RN(SSW+CF) when compared to the Wang data. In this comparison it seems quite likely that MPpredictor benefits from having been trained on the Wang data. This is further demonstrated when we compare the NBS experimental data to the Wang data; a non-negligible discrepancy is seen. This emphasizes that the reference data chosen is an important factor to consider when using, testing and studying a predictive method.

3 Uncertainty estimation



Supplementary Figure 4: Calibration plots of the uncertainty estimators used in the paper for the estimated absolute uncertainties (predicted) against the observed absolute errors (true) for 1550 $\Delta_{\mathrm{f}}H_{\mathrm{r^2SCAN(GGA/GGA+U)-RN(SSW+CF)}}$ predictions. The miscalibration area is represented by the shaded area.

Another correction to the predicted uncertainties can be obtained by minimization of the calibration area via a uniform scaling of all the predicted uncertainties (calibration) [43]. The calibration (cal.) provides significant improvement to the evaluation measures for the SD, but only slight improvement for the MAD. Finally, we can test the serial application of first regression and then calibration (reg.+cal.). Notably, this seems to improve on the individual corrections from regression and calibration w.r.t the MAE, while the miscalibration area is only altered very slightly, in comparison.

Supplementary Table 8: Evaluating uncertainty estimators for 1550 $\Delta_{\mathrm{f}}H_{\mathrm{r^2SCAN(GGA/GGA+U)-RN(SSW+CF)}}$ predictions. The mean absolute error of the estimated uncertainty (MAEU) w.r.t the true absolute errors ($|\Delta_{\mathrm{f}}H_{\mathrm{RN}} - \Delta_{\mathrm{f}}H_{\mathrm{ref}}|$) is given in meV atom^{-1}; a value of zero is ideal. The miscalibration area quantifies systematic under or over-confidence of the predicted uncertainty; a value of zero is ideal. The proportion of reference values within a prediction±1-, ±2- and ±3-times the predicted uncertainty are given under ±1U, ±2U and ±3U, respectively. ρ is Spearman's rank correlation coefficient of the predicted uncertainty and the true absolute errors; a value of one is ideal. The abbreviation reg. means regressed and cal. means calibrated.

Method	MAEU	Miscalibration area	±1U	±2U	±3U	ρ
Constant	27.5	0.08	71%	85%	92%	-
SD (cal.)	24.2	0.04	64%	84%	92%	0.49
MAD (cal.)	23.2	0.03	66%	87%	93%	0.57
SD (reg.+cal.)	22.3	0.05	65%	82%	91%	0.49
MAD (reg.+cal.)	21.1	0.03	64%	85%	92%	0.57

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