

Supplementary Information for: The effects of dispersion damping and three-body interactions for accurate layered material exfoliation energies

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(Dated: May 9, 2026)*

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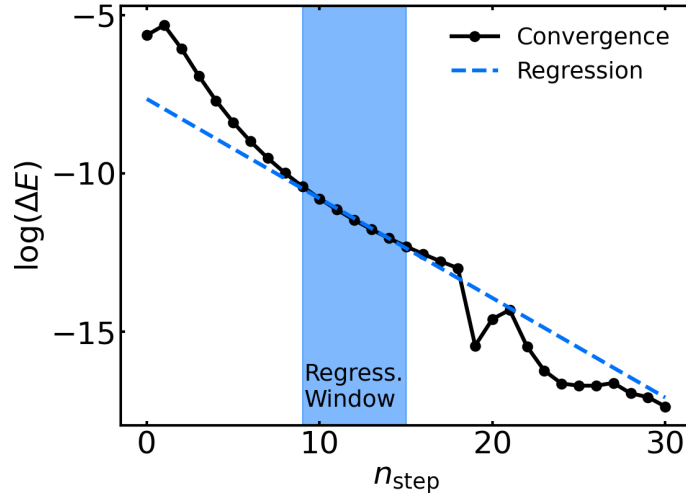


FIG. 1: Visual comparison of direct convergence of the ATM energy *versus* the extrapolation method for a test case: HCP-zirconium.

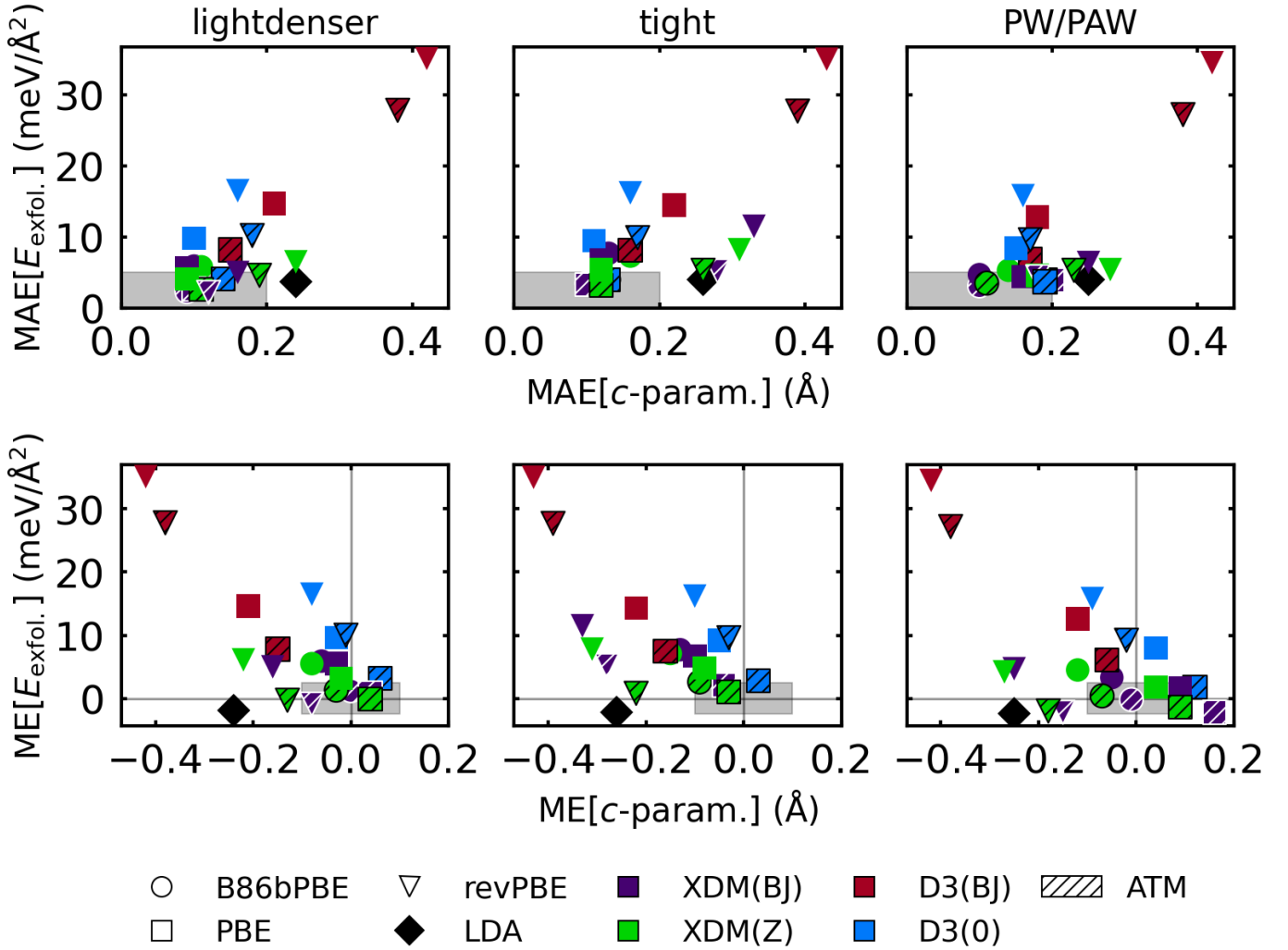


FIG. 2: Plot of the mean absolute errors (MAE) and mean errors (ME) of the exfoliation energies and c -parameters of the LM26 benchmark. A grey box, designating acceptable accuracy of $5 \text{ meV}/\text{\AA}^2$ for $E_{\text{exfol.}}$ and 0.2 \AA for c -parameters, is also shown.

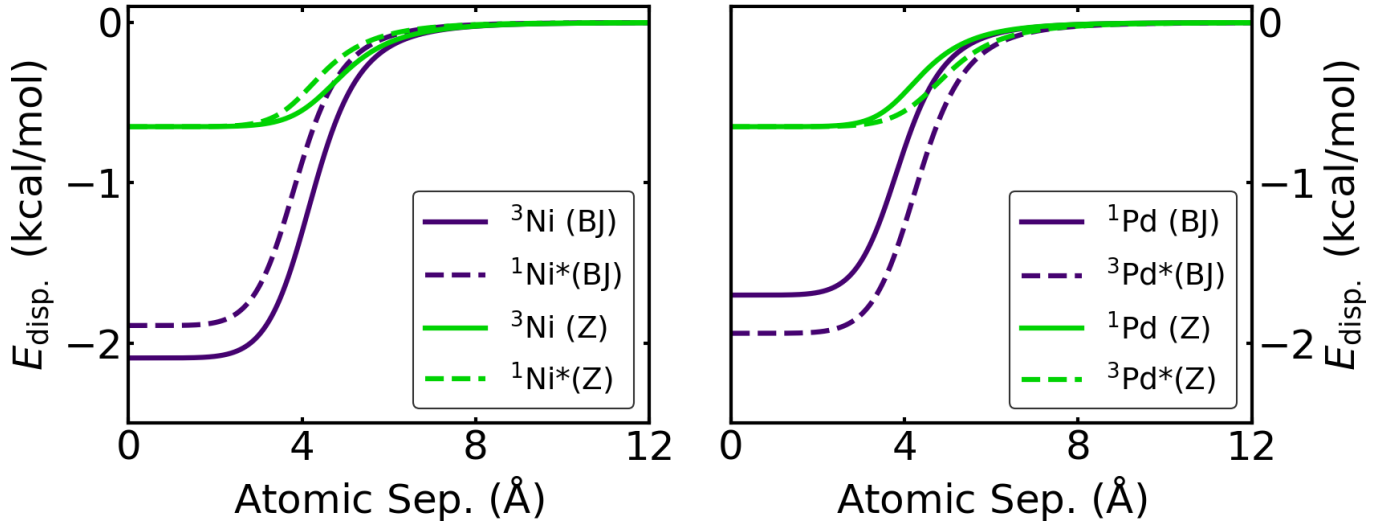


FIG. 3: Comparison of the BJ- and Z-damping functions for singlet and triplet nickel and palladium. All calculations used the same methodology as described in Figure 2 of the main text.

TABLE I: Reference data used for the LM26 benchmark.

LM	$c_{\text{ref.}}$ (Å)	$ab\text{-area}$ (Å ²)	n_{layers}	$E_{\text{ref.}}^{\text{RPA}}$ (meV/Å ²)	$E_{\text{ref.}}^{\text{RPA}}$ (kcal/mol/layer)
BN	6.7	5.5	2	21.6	2.7
graphite	6.9	5.3	2	19.7	2.4
HfS ₂	5.8	11.4	1	16.1	4.2
HfSe ₂	6.2	12.2	1	17.1	4.8
HfTe ₂	6.7	13.6	1	18.7	5.8
MoS ₂	12.3	8.7	2	20.5	4.1
MoSe ₂	12.9	9.4	2	19.6	4.2
MoTe ₂	14.0	10.7	2	20.8	5.1
NbSe ₂	12.5	10.3	2	19.6	4.6
NbTe ₂	6.6	11.7	1	23.0	6.2
PbO	5.0	15.8	1	20.2	7.3
PdTe ₂	5.1	14.1	1	40.2	13.0
PtS ₂	5.0	10.9	1	20.6	5.2
PtSe ₂	5.1	12.0	1	19.1	5.3
TaS ₂	5.9	9.8	1	17.7	4.0
TaSe ₂	6.2	10.7	1	19.4	4.8
TiS ₂	5.7	10.0	1	18.9	4.3
TiSe ₂	6.0	10.9	1	17.4	4.3
TiTe ₂	6.5	12.2	1	19.8	5.6
VS ₂	5.8	9.0	1	25.6	5.3
VSe ₂	6.0	9.7	1	22.3	5.0
WS ₂	12.3	8.7	2	20.2	4.0
WSe ₂	13.0	9.3	2	20.0	4.3
ZrS ₂	5.8	11.6	1	17.0	4.5
ZrSe ₂	6.1	12.3	1	18.5	5.2
ZrTe ₂	6.7	13.5	1	16.3	5.1

TABLE II: Mean absolute errors (MAE) and mean errors (ME) in kcal/mol per layer for the LM26 benchmark of exfoliation energies of 26 layered materials, including graphite, boron nitride, lead(II) oxide, and transition-metal dichalcogenides.

Functional	lightdenser		tight		PW	
	MAE	ME	MAE	ME	MAE	ME
revPBE-D3(BJ)	8.8	8.8	8.8	8.8	8.6	8.6
revPBE-D3(BJ)+ATM	7.0	7.0	7.0	7.0	6.9	6.9
revPBE-D3(0)	4.1	4.1	4.1	4.1	4.0	4.0
revPBE-D3(0)+ATM	2.6	2.5	2.5	2.5	2.4	2.4
PBE-D3(BJ)	3.7	3.7	3.7	3.7	3.3	3.2
PBE-D3(BJ)+ATM	2.1	2.0	2.1	2.0	1.8	1.6
PBE-D3(0)	2.5	2.4	2.4	2.4	2.1	2.1
PBE-D3(0)+ATM	1.0	0.9	1.0	0.8	0.9	0.5
revPBE-XDM(BJ)	1.3	1.3	2.9	2.9	1.6	1.2
revPBE-XDM(Z)	1.8	1.7	2.3	2.2	1.5	1.2
revPBE-XDM(BJ)+ATM	0.5	-0.2	1.4	1.4	1.1	-0.5
revPBE-XDM(Z)+ATM	1.2	0.1	1.4	0.4	1.3	-0.4
B86bPBE-XDM(BJ)	1.5	1.5	2.0	2.0	1.2	0.8
B86bPBE-XDM(Z)	1.6	1.5	2.0	1.9	1.4	1.2
B86bPBE-XDM(BJ)+ATM	0.6	0.4	0.9	0.9	0.8	-0.0
B86bPBE-XDM(Z)+ATM	0.8	0.5	1.1	0.8	0.9	0.2
PBE-XDM(BJ)	1.5	1.5	1.8	1.8	1.2	0.5
PBE-XDM(Z)	1.1	0.9	1.4	1.3	1.2	0.6
PBE-XDM(BJ)+ATM	0.7	0.3	0.9	0.6	1.0	-0.5
PBE-XDM(Z)+ATM	0.6	0.1	0.8	0.4	0.9	-0.2
revPBE	4.9	-4.9	5.0	-5.0	5.0	-5.0
B86bPBE	4.6	-4.6	4.7	-4.7	4.8	-4.8
PBE	4.3	-4.3	4.5	-4.5	4.6	-4.6
PBEsol	2.8	-2.8	2.8	-2.8	3.0	-3.0
LDA	0.8	-0.3	0.9	-0.4	0.9	-0.4

TABLE III: Mean absolute errors (MAE) and mean errors (ME) in Ångströms for the LM26 benchmark of c -parameters of 26 layered materials, including graphite, boron nitride, lead(II) oxide, and transition-metal dichalcogenides.

Functional	lightdenser		tight		PW	
	MAE	ME	MAE	ME	MAE	ME
revPBE-D3(BJ)	0.42	-0.42	0.43	-0.43	0.42	-0.42
revPBE-D3(BJ)+ATM	0.38	-0.38	0.39	-0.39	0.38	-0.38
revPBE-D3(0)	0.16	-0.08	0.16	-0.10	0.16	-0.09
revPBE-D3(0)+ATM	0.18	-0.01	0.17	-0.03	0.17	-0.02
PBE-D3(BJ)	0.21	-0.21	0.22	-0.22	0.18	-0.12
PBE-D3(BJ)+ATM	0.15	-0.15	0.16	-0.16	0.17	-0.06
PBE-D3(0)	0.10	-0.03	0.11	-0.05	0.15	0.04
PBE-D3(0)+ATM	0.14	0.06	0.13	0.03	0.19	0.12
revPBE-XDM(BJ)	0.16	-0.16	0.33	-0.33	0.25	-0.25
revPBE-XDM(Z)	0.24	-0.22	0.31	-0.31	0.28	-0.27
revPBE-XDM(BJ)+ATM	0.12	-0.08	0.28	-0.28	0.18	-0.15
revPBE-XDM(Z)+ATM	0.19	-0.13	0.26	-0.22	0.23	-0.18
B86bPBE-XDM(BJ)	0.10	-0.06	0.13	-0.13	0.10	-0.05
B86bPBE-XDM(Z)	0.11	-0.08	0.16	-0.15	0.14	-0.12
B86bPBE-XDM(BJ)+ATM	0.09	0.00	0.10	-0.08	0.10	-0.01
B86bPBE-XDM(Z)+ATM	0.10	-0.03	0.13	-0.09	0.11	-0.07
PBE-XDM(BJ)	0.09	-0.03	0.12	-0.10	0.16	0.09
PBE-XDM(Z)	0.09	-0.02	0.12	-0.08	0.18	0.04
PBE-XDM(BJ)+ATM	0.10	0.04	0.10	-0.04	0.20	0.16
PBE-XDM(Z)+ATM	0.11	0.04	0.12	-0.03	0.19	0.09
revPBE	2.90	2.90	3.50	3.50	3.82	3.82
B86bPBE	1.25	1.25	1.38	1.38	1.68	1.68
PBE	1.02	1.02	1.02	1.02	1.17	1.17
PBEsol	0.13	0.01	0.15	0.00	0.16	0.00
LDA	0.24	-0.24	0.26	-0.26	0.25	-0.25

TABLE IV: Minimum (MIN), maximum (MAX), and mean (AVG) values of the ATM term with various damping schemes in meV/Å² for the LM26 benchmark.

Method		lightdenser			tight			PW		
		MIN	MAX	AVG	MIN	MAX	AVG	MIN	MAX	AVG
revPBE	ATM(0)	2.5	11.6	6.6	2.4	11.6	6.6	2.4	11.5	6.6
	ATM(BJ)	2.6	7.9	5.9	3.0	8.3	6.3	1.7	10.0	6.9
	ATM(Z)	2.8	8.6	6.4	3.1	9.5	7.0	-0.5	6.3	6.3
B86bPBE	ATM(BJ)	1.8	6.2	4.7	1.9	6.0	4.5	0.1	5.3	3.5
	ATM(Z)	1.5	5.5	4.2	1.6	6.2	4.6	1.6	5.2	4.1
PBE	ATM(0)	2.7	10.4	6.4	2.7	10.3	6.4	2.8	9.2	6.3
	ATM(BJ)	1.5	6.3	4.6	1.5	6.3	4.6	-0.3	5.6	3.9
	ATM(Z)	1.1	4.5	3.4	1.2	5.1	3.7	1.2	4.4	3.2

TABLE V: Minimum (MIN), maximum (MAX), and mean (AVG) values of the ATM term with various damping schemes in kcal/mol per layer for the LM26 benchmark.

Method		lightdenser			tight			PW		
		MIN	MAX	AVG	MIN	MAX	AVG	MIN	MAX	AVG
revPBE	ATM(0)	0.5	2.9	1.6	0.5	2.9	1.6	0.5	2.9	1.6
	ATM(BJ)	0.3	2.1	1.5	0.4	2.2	1.6	0.4	2.3	1.7
	ATM(Z)	0.4	2.3	1.6	0.4	2.6	1.8	-0.1	4.4	1.7
B86bPBE	ATM(BJ)	0.2	1.7	1.2	0.2	1.6	1.1	0.0	1.1	0.8
	ATM(Z)	0.2	1.5	1.0	0.2	1.7	1.1	0.2	1.4	1.0
PBE	ATM(0)	0.4	2.6	1.6	0.4	2.6	1.6	0.4	2.7	1.5
	ATM(BJ)	0.2	1.7	1.1	0.2	1.7	1.1	-0.1	1.4	0.9
	ATM(Z)	0.1	1.2	0.8	0.1	1.4	0.9	0.1	1.2	0.8