Transferable Dispersion-Aware Machine Learning Interatomic Potentials Potentials for Few-Layer Transition Metal Dichalcogenide Heterostructures

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	system	Train set	Test set
Monolayer	WS_2	1786	213
	WSe_2	2247	253
	MoS_2	1982	244
	$MoSe_2$	2262	238
	$MoTe_2$	1238	148
	hBN	1138	0
Homobilayer	MoS_2/MoS_2	5469	578
	$MoSe_2/MoSe_2$	5183	577
	$MoTe_2/MoTe_2$	4610	520
	WS_2/WS_2	5463	598
	WSe_2/WSe_2	5220	531
Heterobilayer	$MoS_2/MoSe_2$	5590	577
	$MoS_2/MoTe_2$	1608	190
	MoS_2/WS_2	5722	638
	MoS_2/WSe_2	10628	1221
	$MoTe_2/WS_2$	2995	355
	$MoTe_2/WSe_2$	4213	445
	$MoSe_2/MoTe_2$	3758	424
	$MoSe_2/WSe_2$	5160	536
	WS_2/WSe_2	5666	655
Monolayer/hBN	MoS_2/hBN	325	0
	$MoSe_2$/hBN	330	0
	$MoTe_2$/hBN	307	0
	WS_2/hBN	429	0
	WSe_2/hBN	330	0
	total	83659	8941

TABLE I. The training and test dataset per system as generated through the active learning procedure.

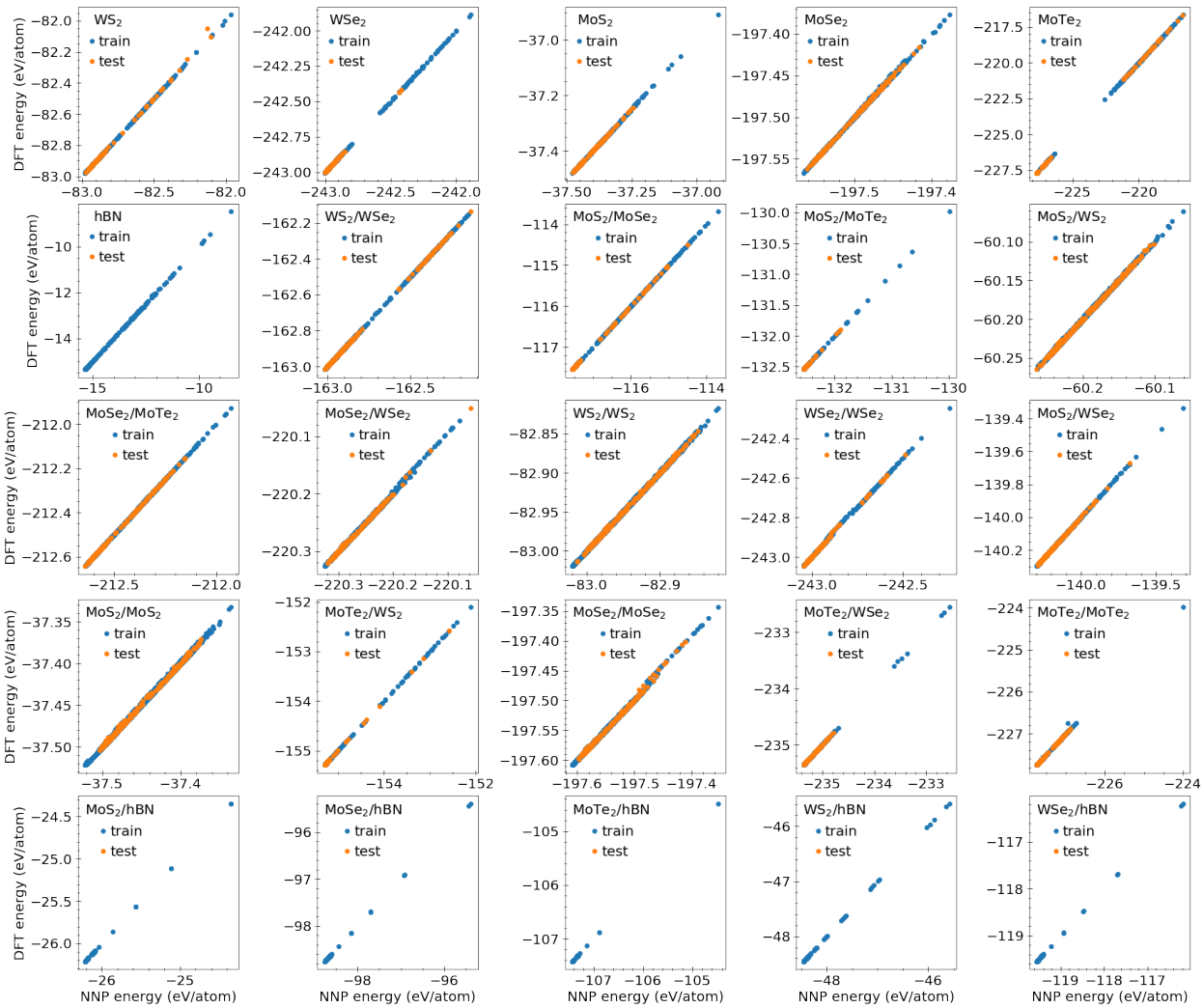

FIG. 1. DFT versus NNP energy correlation decomposed into the different systems in the training dataset

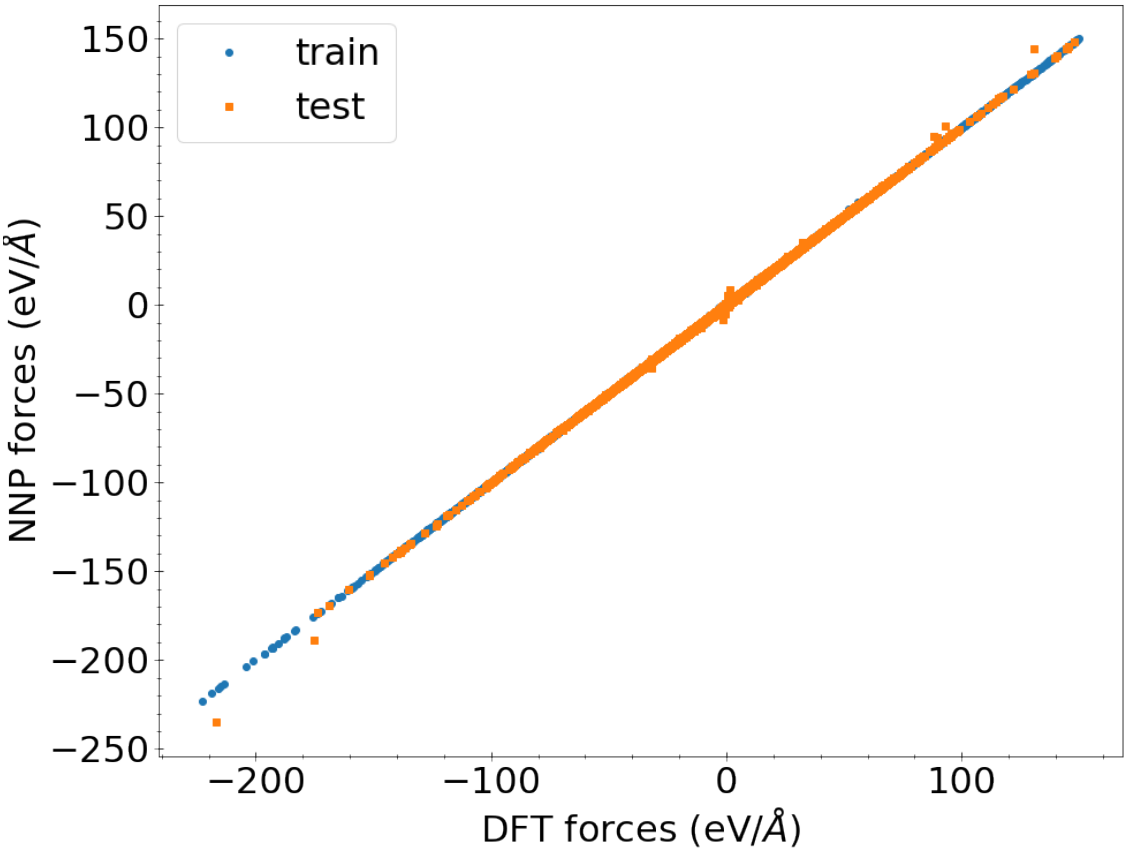

FIG. 2. DFT versus NNP force components correlation

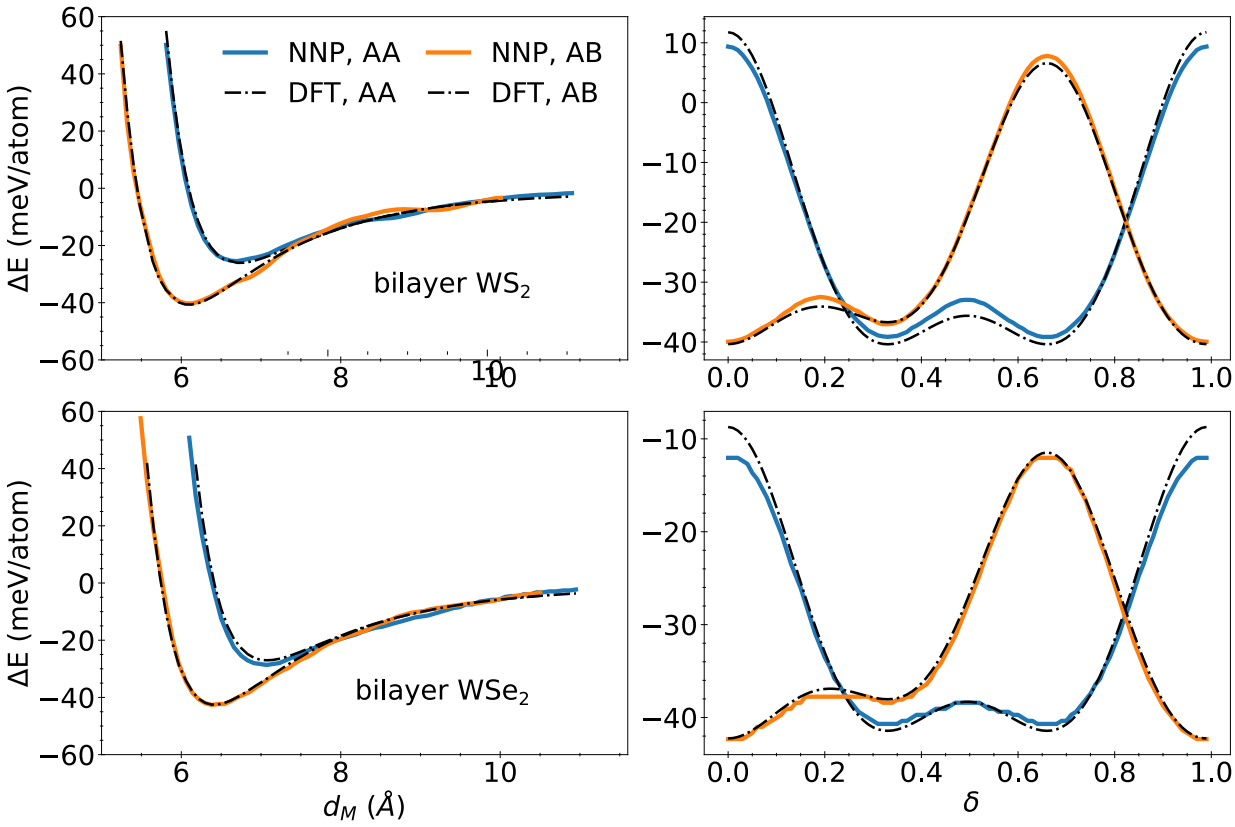

FIG. 3. Bilayer interlayer binding and sliding energy for WS_2 and WSe_2. δ is in unit of the cell size

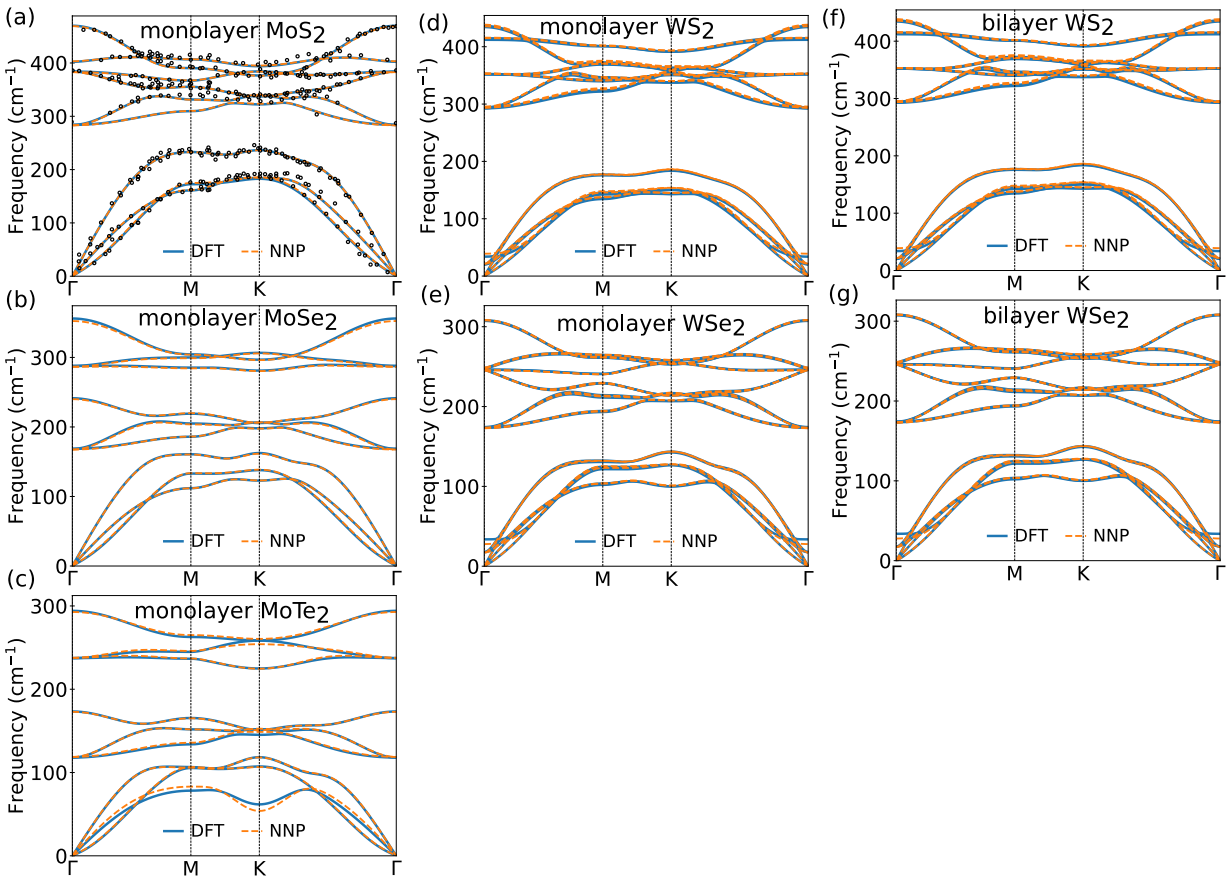

FIG. 4. Vibrational frequencies for monolayer TMDs (a) MoS_2 (b) $MoSe_2$ and (c) $MoTe_2$ (d) WS_2 (e)WSe_2; and bilayer TMDs (f) WS_2 and (g) WSe_2

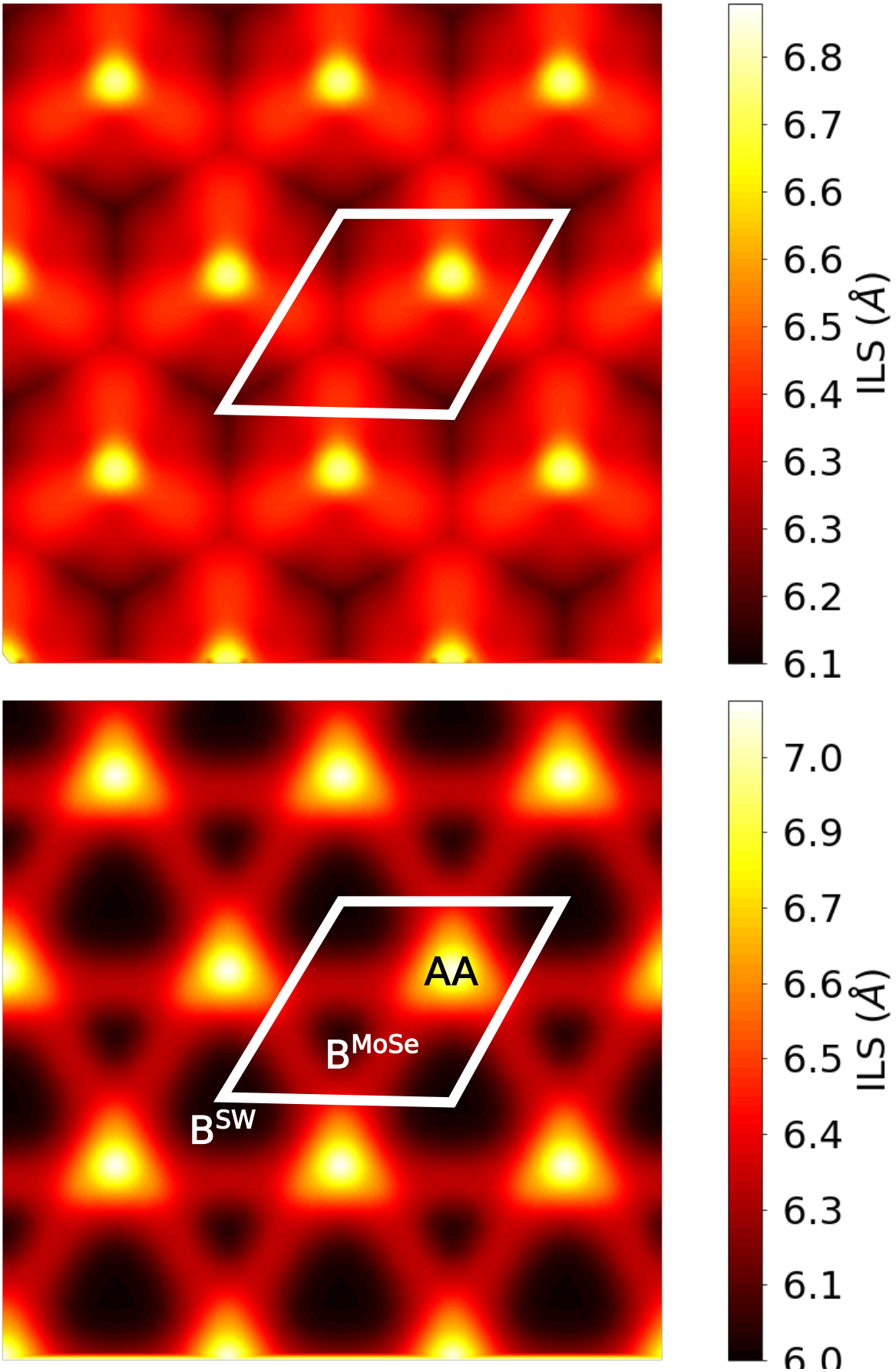

FIG. 5. Mo-W interlayer spacing without hBN and with hBN substrate respectively