Supplementary Material

Physics infused machine learning force fields for 2D materials monolayers

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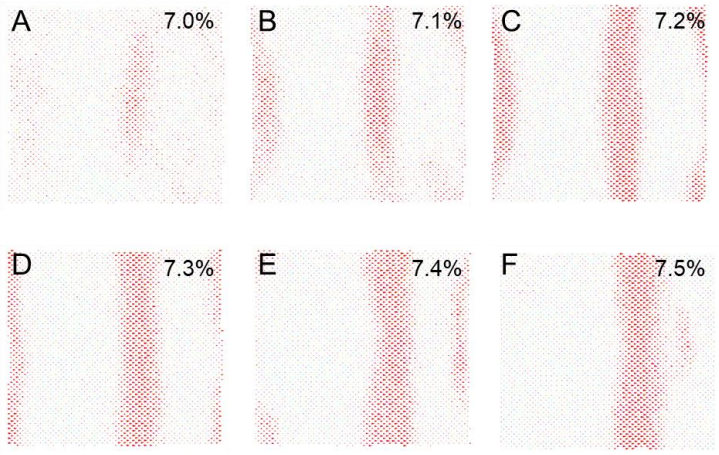
Supplementary Table 1. Comparison the fitting quality by using different adjustable parameters

		original	**0.1η**	**10η**	**0.1k**	**10:q**
GeSe	RMSE (eV/atom)	1.530	5.533	2.171	1.633	2.143
	MAE (eV/atom)	1.060	3.674	1.488	1.150	1.434
	R^2	0.998	0.975	0.996	0.998	0.996
PbTe	RMSE (eV/atom)	0.920	8.337	1.353	0.920	1.426
	MAE (eV/atom)	0.640	5.526	0.977	0.628	0.976
	R^2	0.999	0.923	0.998	0.999	0.998
*h*BN	RMSE (eV/atom)	0.840	1.004	0.773	0.625	0.660
	MAE (eV/atom)	0.400	0.546	0.405	0.313	0.329
	R^2	0.9999	0.9997	0.9998	0.9999	0.9999

Supplementary Table 2. Formation energy of point defects in monolayer GeSe, PbTe and *h*BN

Formation energy		**DFT**	**ML**	**Relative error**
Vacancy	$E_{\mathrm{V}}^{\mathrm{Ge}}$	5.874	4.674	20.4%
	$E_{\mathrm{V}}^{\mathrm{Se}}$	5.879	4.912	16.4%
	$E_{\mathrm{V}}^{\mathrm{Pb}}$	5.564	4.231	23.9%
	$E_{\mathrm{V}}^{\mathrm{Te}}$	4.864	5.280	8.5%
	$E_{\mathrm{V}}^{\mathrm{B}}$	16.564	15.552	6.1%
	$E_{\mathrm{V}}^{\mathrm{N}}$	16.020	21.211	32.4%
Anti-sites	E_{GeSe}^{1}	1.476	1.138	22.9%
	E_{GeSe}^{2}	2.522	2.486	1.4%
	E_{PbTe}^{1}	2.112	3.358	59.0%
	E_{PbTe}^{2}	2.567	2.504	2.4%
	$E_{h\mathrm{BN}}$	7.585	9.360	23.4%
Domain boundary (eV/nm)	GeSe	0.791	0.603	23.7%
Phase boundary (eV/nm)	PbTe	4.467	1.124	74.8%
Grain boundary (eV/nm)	*h*BN	5.967	6.740	12.9%



Supplementary Figure 1. Typical atomic configurations of monolayer PbTe during a stress induced phase transformation at 50 K. (A)-(C) Ferroic phase grows up by the movement of the phase boundary during a typical stress drop from ε = 7.0% to ε = 7.2%; (D)-(F) Ferroic phase shrinks by the movement of the phase boundary during a typical stress increment from ε = 7.3% to ε = 7.5%.