Supporting Information: Evolutionary exploration of polytypism in lead halide perovskites

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Table S1: Comparison of ordering energies for unseen polytypes calculated from DFT and using the pre-trained model Hamiltonian (total energy in eV; ordering energy in meV/layer).

New polytypes	$E_{Total,DFT}$	$E_{Total,Model}$	$E_{Ordering,DFT}$	$E_{Ordering,Model}$
11H(3c8h)-$CsPbI_3$	-135.243	-134.766	30.8	74.2
11H(3c8h)-$CsPbBr_3$	-154.256	-154.371	45.8	35.4
18H(1h8c1h8c)-$CsPbI_3$	-220.376	-220.343	82.6	84.4