Supplementary Materials

Data-driven strategy for bandgap database construction of perovskites and the potential segregation study

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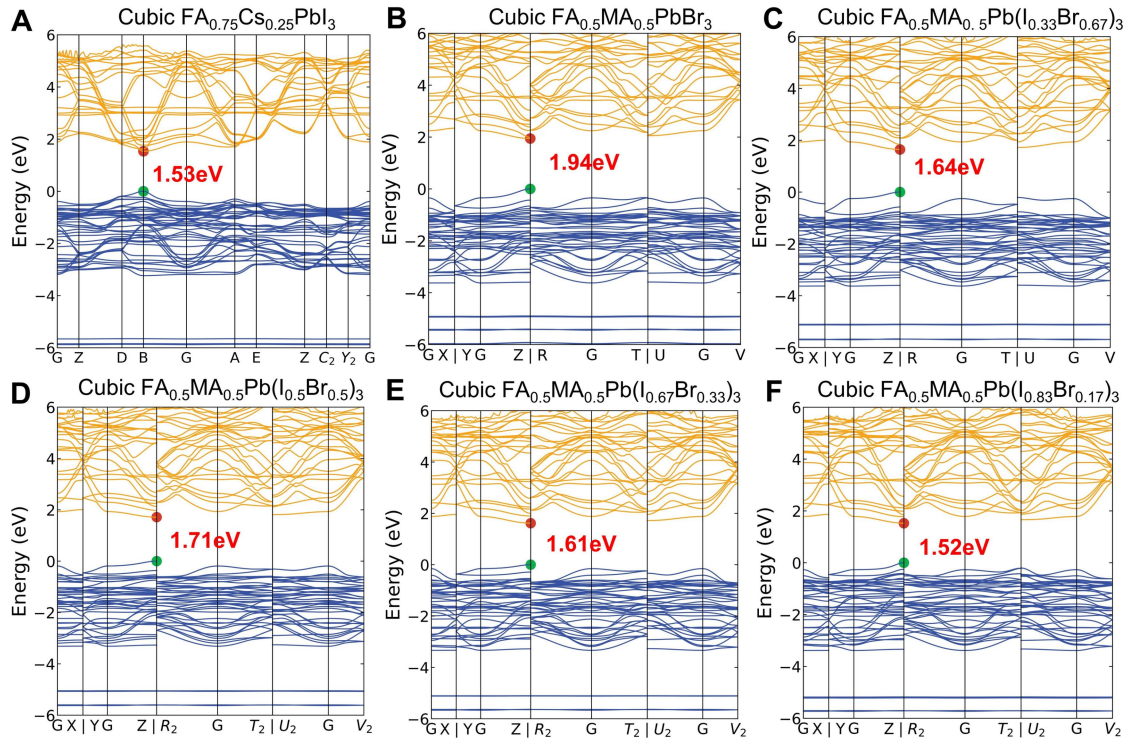
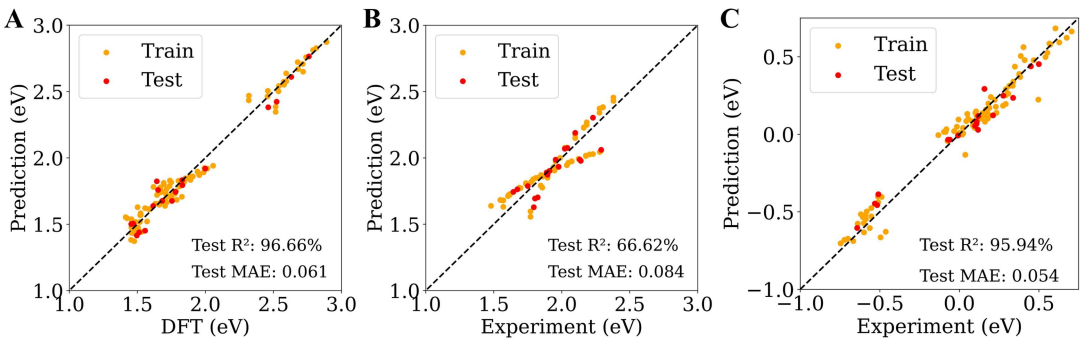
Supplementary Table 1. Formulas for the bandgap in eV as a function of relative Br concentration x for the five compounds

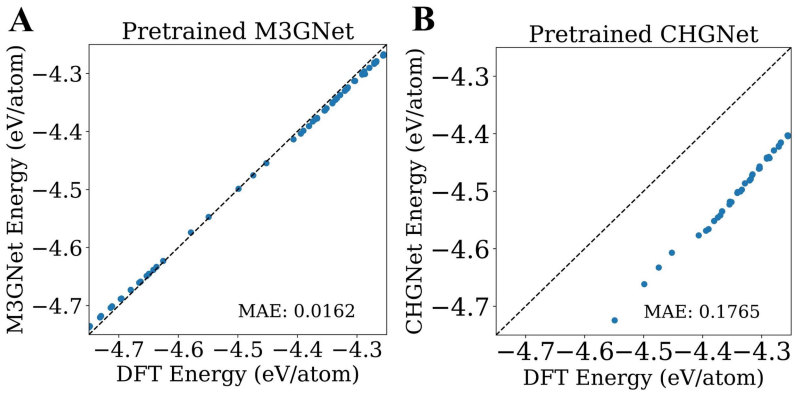
Compounds	Bandgap	Ref
Cubic $FAPb(I_{1-x}Br_x)_3$	$1.48(1 - x) + 2.23x - 0.15x(1 - x)$	[1]
Cubic $MAPb(I_{1-x}Br_x)_3$	$1.57(1 - x) + 2.29x - 0.33x(1 - x)$	[2]
Cubic $CsPb(I_{1-x}Br_x)_3$	$1.77(1 - x) + 2.38x - 0.35x(1 - x)$	[3]
Tetragonal $MAPb(I_{1-x}Br_x)_3$	$1.57(1 - x) + 2.25x - 0.3x(1 - x)$	[4]
Orthorhombic $CsPb(I_{1-x}Br_x)_3$	$1.73(1 - x) + 2.34x - 0.22x(1 - x)$	[5]



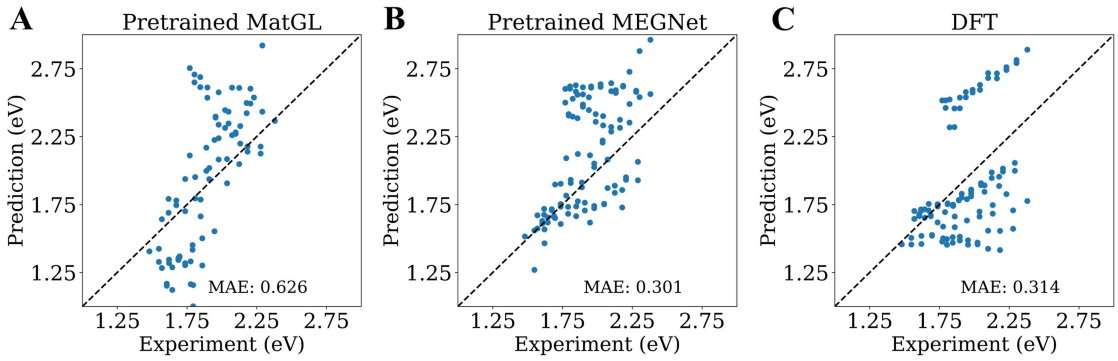
Supplementary Figure 1. DFT calculated electronic band structures for six representative mixed halide perovskites in cubic structure. (A) $FA_{0.75}Cs_{0.25}PbI_3$; (B) $FA_{0.5}MA_{0.5}PbBr_3$; (C) $FA_{0.5}MA_{0.5}Pb(I_{0.33}Br_{0.67})_3$; (D) $FA_{0.5}MA_{0.5}Pb(I_{0.5}Br_{0.5})_3$; (E) $FA_{0.5}MA_{0.5}Pb(I_{0.67}Br_{0.33})_3$; (F) $FA_{0.5}MA_{0.5}Pb(I_{0.83}Br_{0.17})_3$.



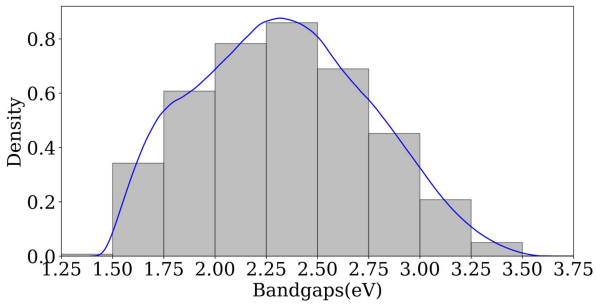
Supplementary Figure 2. Performances of fine-tuned MEGNet in different datasets. (A) DFT bandgap dataset; (B) The experimental bandgap dataset; (C) The gap between experimental and DFT bandgap dataset.



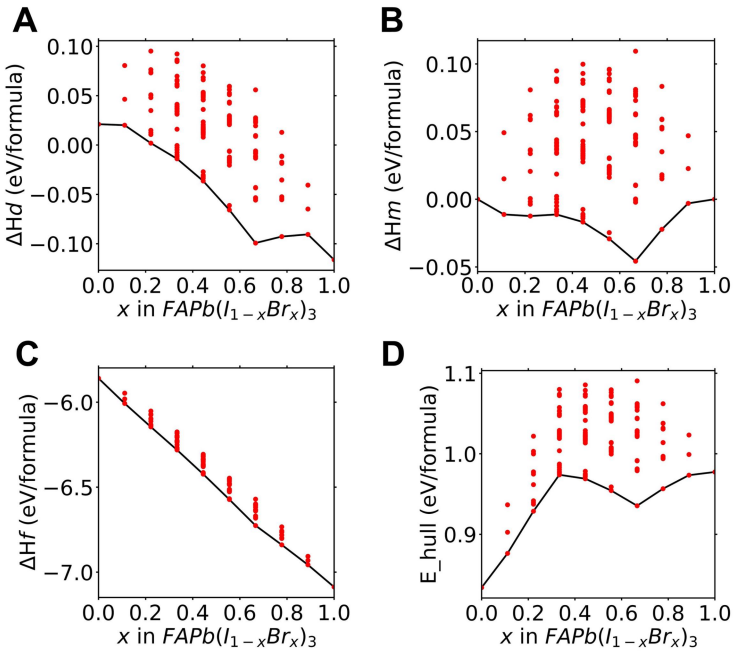
Supplementary Figure 3. Total energy prediction results of different graph neural networks. (A) M3GNet; (B) CHGNet.



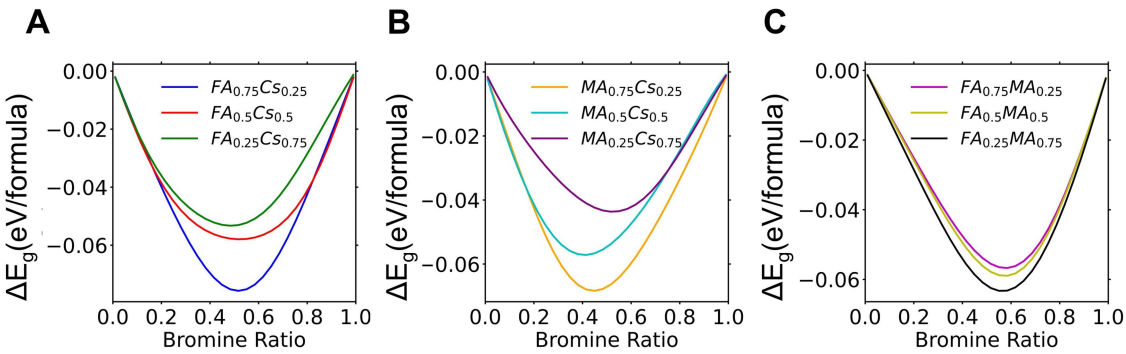
Supplementary Figure 4. Prediction results of different methods in DFT bandgap dataset. (A) Pretrained MatGL; (B) Pretrained MEGNet; (C) DFT method.



Supplementary Figure 5. The probability density distribution of perovskite bandgap database.



Supplementary Figure 6. (A) Decomposition energy; (B) Mixing energy; (C) Formation energy; (D) Energy above hull of $FAPb(I_{1-x}Br_x)_3$.



Supplementary Figure 7. ΔE_g for the different compounds ($APb(I_{1-x}Br_x)_3$). A = (A) $FA_{0.75}Cs_{0.25}$, $FA_{0.5}Cs_{0.5}$ and $FA_{0.25}Cs_{0.75}$; (B) $MA_{0.75}Cs_{0.25}$, $MA_{0.5}Cs_{0.5}$ and $MA_{0.25}Cs_{0.75}$; (C) $FA_{0.75}MA_{0.25}$, $FA_{0.5}MA_{0.5}$ and $FA_{0.25}MA_{0.75}$.

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