Structural and electronic properties of hybrid organo-halide perovskites
from first principle molecular dynamics

Supplementary Information

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Figure SI1. Theoretical XRD patterns obtained on the average structure of the MA β1, 2 and 3 models, compared with the experimental data.
Figure S12. Average of all the I-Pb-Pb-I dihedral angles within the reference cell, without sign, calculated along the three pseudo-cubic directions for the investigated structures.
Figure SI3. Evolution of the orientation of an arbitrary chosen MA cation in the MA $\alpha$ structure.
Figure SI4. Comparison between the Theoretical and experimental electronic Density of States (DOS), reported in Ref. 52 and the theoretical DOS computed for the MA $\beta_{1,2,3}$ and for the FA $\alpha$ system. Our DOS are shifted to match the data range reported in Ref. 52. A broadening of 0.01 eV is used in our calculations.
References