Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

Supplementary Information

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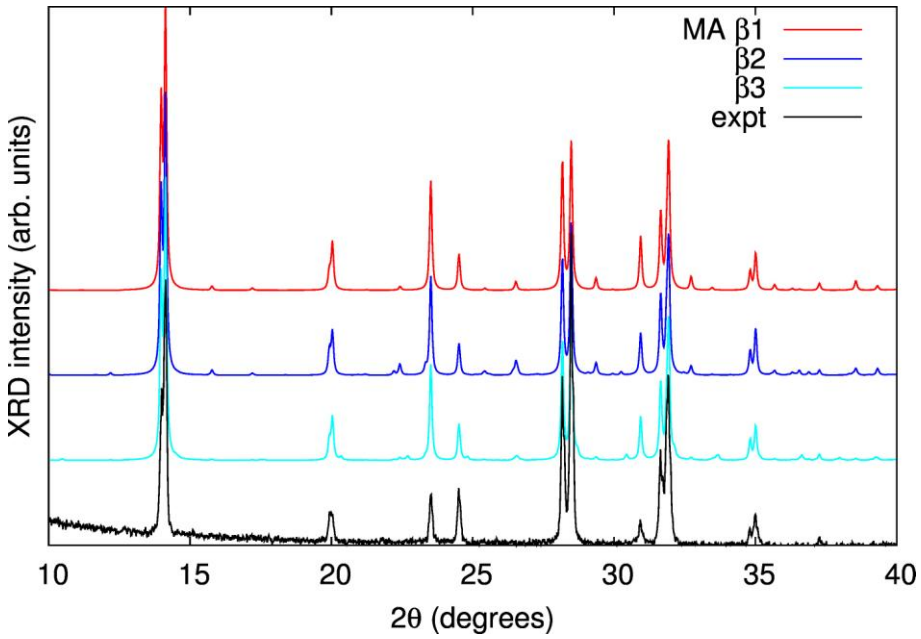

Figure SI1. Theoretical XRD patterns obtained on the average structure of the MA β1, 2 and 3 models, compared with the experimental data.

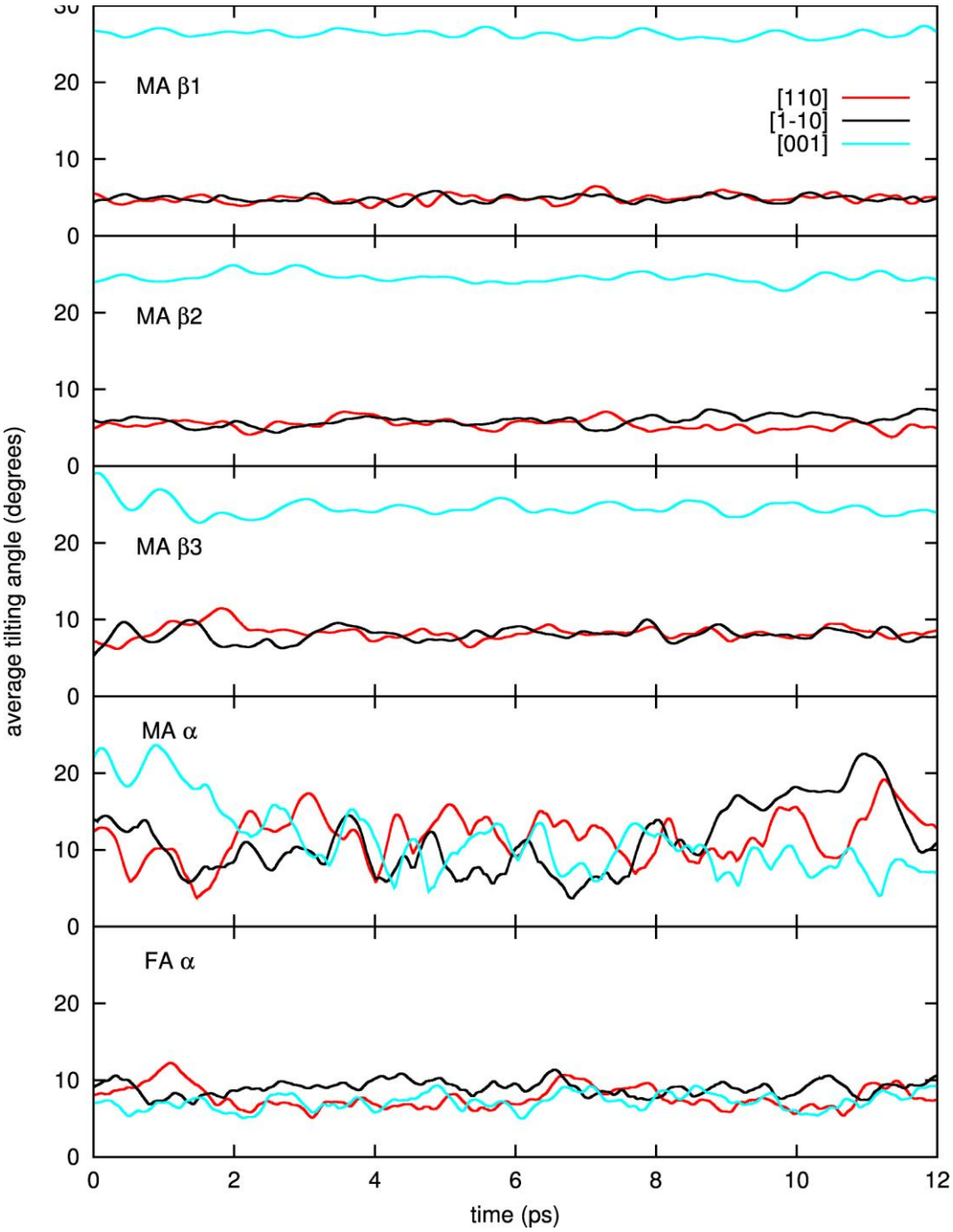

Figure SI2. Average of all the I-Pb-Pb-I dihedral angles within the reference cell, without sign, calculated along the three pseudo-cubic directions for the investigated structures.

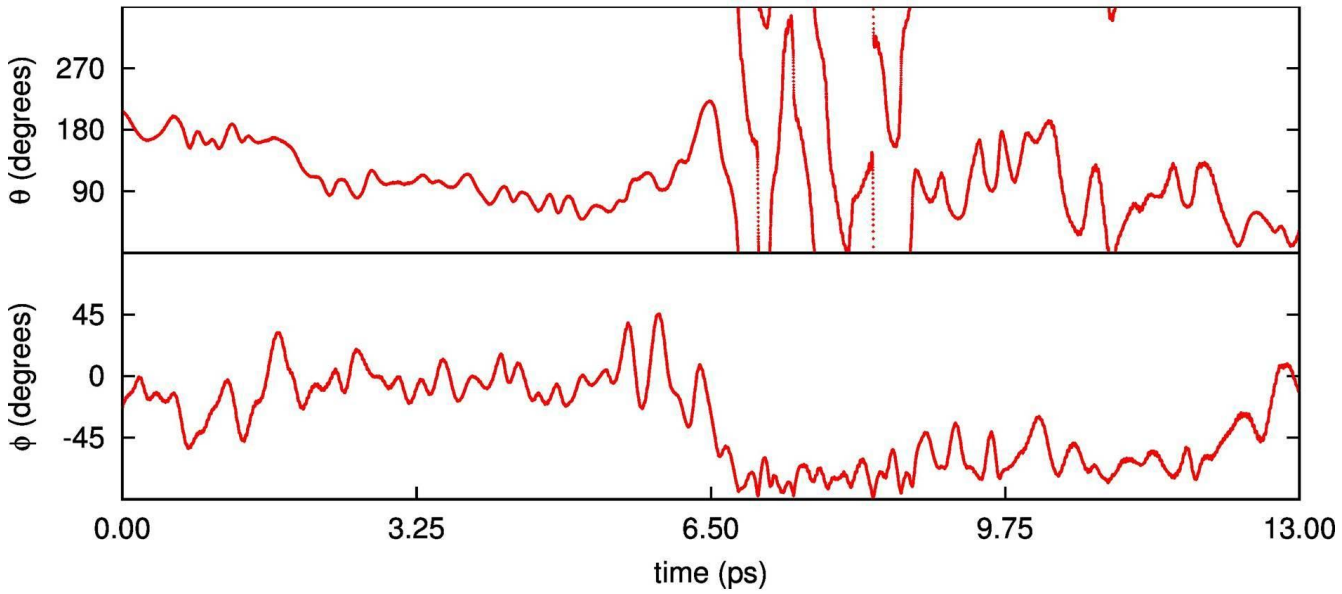

Figure SI3. Evolution of the orientation of an arbitrary chosen MA cation in the MA α structure.

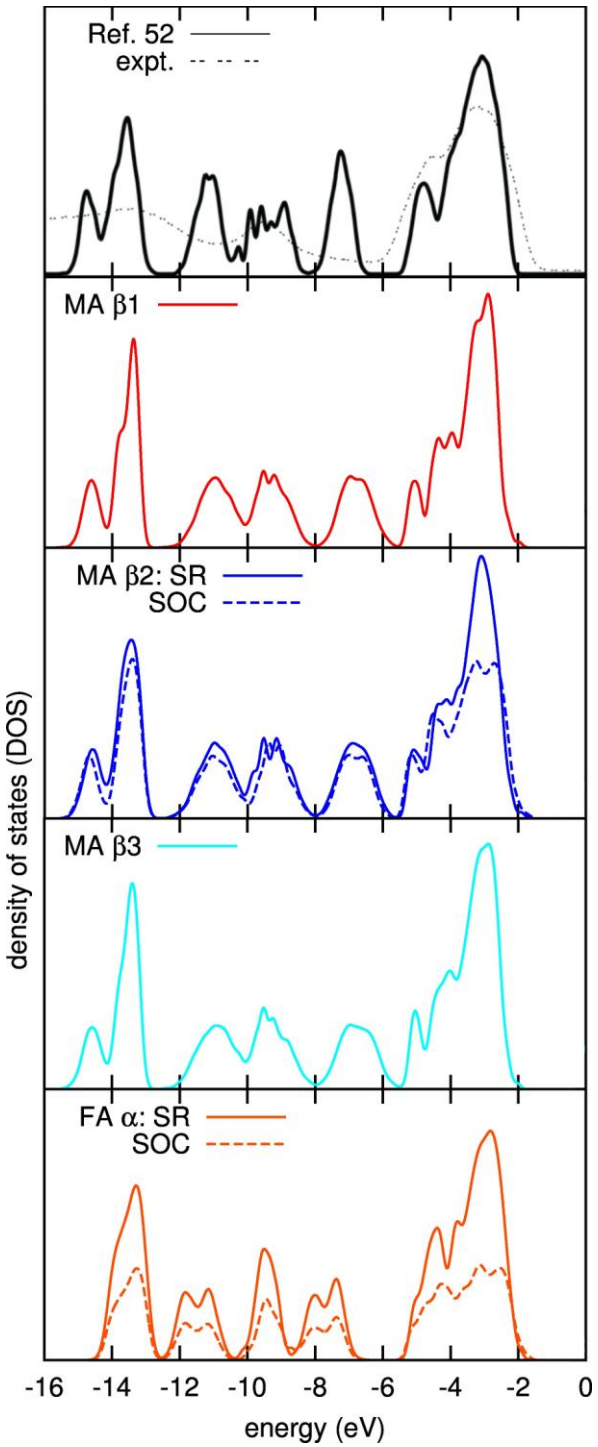

Figure SI4. Comparison between the Theoretical and experimental electronic Density of States (DOS), reported in Ref. 52 and the theoretical DOS computed for the MA β1,2,3 and for the FA α system. Our DOS are shifted to match the data range reported in Ref. 52. A broadening of 0.01 eV is used in our calculations.

References

1. A. Poglitsch and D. Weber, Dynamic Disorder in Methyl-ammoniumtrihalogenoplumbates(II) Observed by Millime-terwave Spectroscopy, *J. Chem. Phys.*, 1987, **87**, 6373–6378.