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

Supplementary information for publication: Effect of the magnitude and direction of the dipole of the organic cation on the electronic structure of hybrid halide perovskites

Sudeep Maheshwari,[†] Sameer Patwardhan,[‡] George C. Schatz,[‡] Nicolas Renaud,[¶] and Ferdinand C. Grozema[*,†]

[†]*Department of Chemical Engineering, Delft University of Technology, P.O. Box 5045, 2629 HZ Delft, The Netherlands*

[‡]*Argonne-Northwestern Solar Energy Research (ANSER) Center and Department of Chemistry, Northwestern University, Evanston, Illinois 60208-3113, United States*

[¶]*Netherlands eScience Center, Science Park 140 1098 XG Amsterdam, The Netherlands*

E-mail: f.c.grozema@tudelft.nl

Figure 1 shows the relaxed geometries of parallel and anti-parallel oriented methylammonium cation along with the plot of respective bandstructures. As seen here, there is little effect of relaxation on the electronic properties of the material.

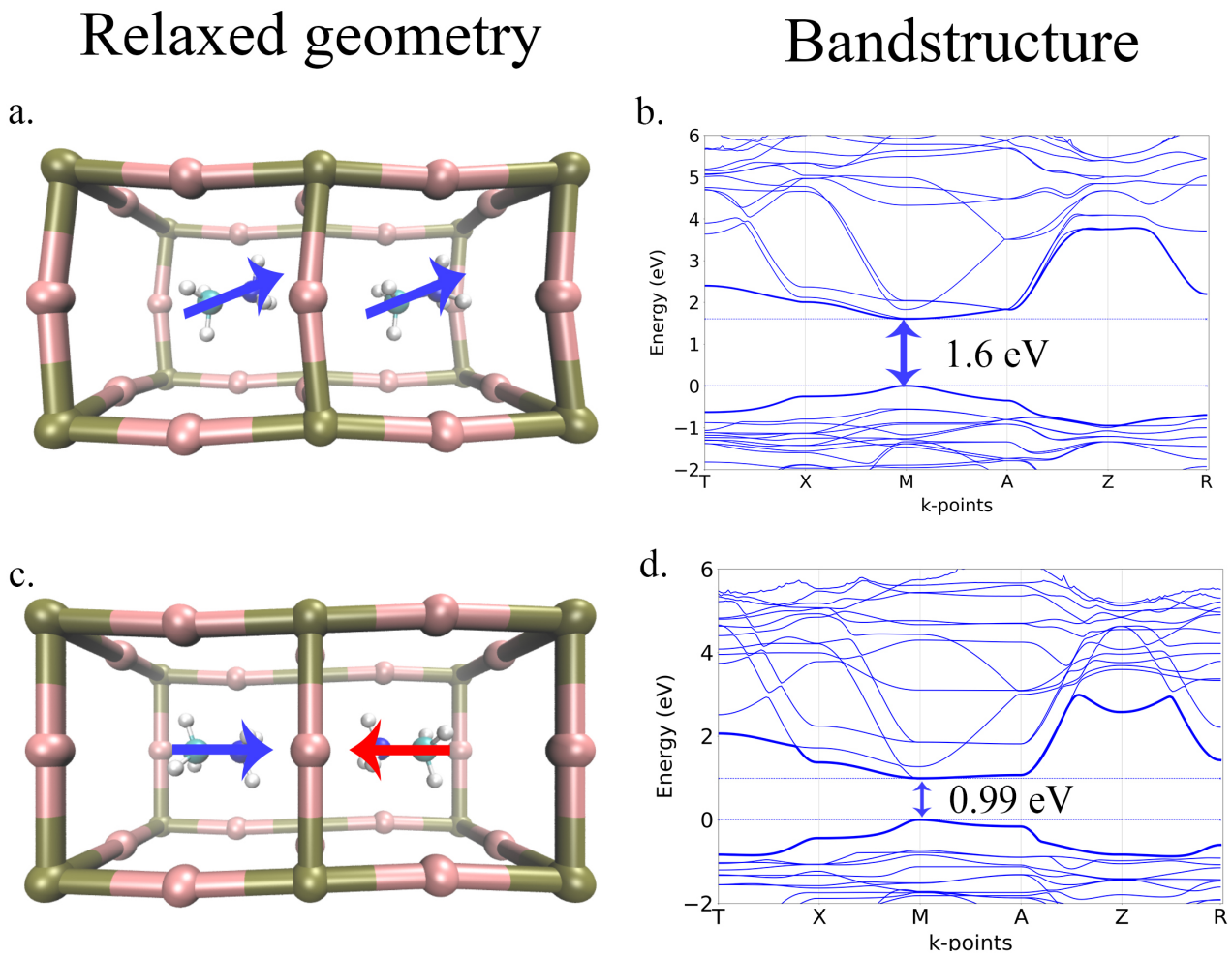

Figure 1: (a) The relaxed geometry for parallel orientation of $MAPbI_3$, (b) Band structure in parallel orientation of dipoles, (c) The relaxed geometry for anti-parallel orientation of $MAPbI_3$ and (d) Band structure in anti-parallel orientation of dipoles. The k-points in Brillouin zone are $T : [0, 0, 0], X : [0, 0, \frac{1}{2}], M : [0, \frac{1}{2}, \frac{1}{2}], A : [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}], Z : [\frac{1}{2}, 0, 0], R : [\frac{1}{2}, 0, \frac{1}{2}]$