First Principles Investigation of the TiO_2/Organohalide Perovskites Interface: The Role of Interfacial Chlorine

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SUPPORTING INFORMATION

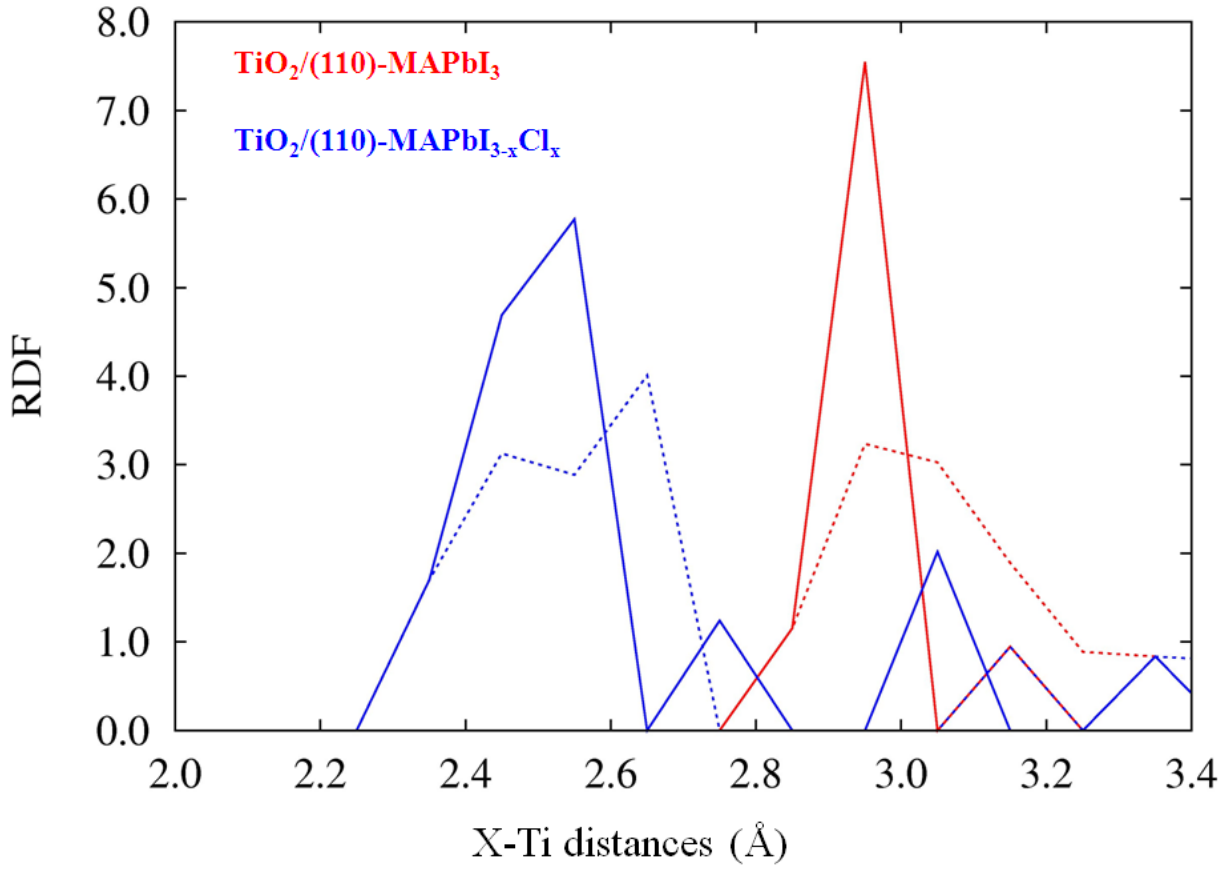

Figure S1. X-Ti (X=I or Cl) radial distribution functions (RDF) for the $TiO_2/MAPbI_3$ (red) and $TiO_2/MAPbI_{3-x}Cl_x$ (blue) interfaces. Solid and dashed lines correspond to the (110) and (001) surfaces, respectively.

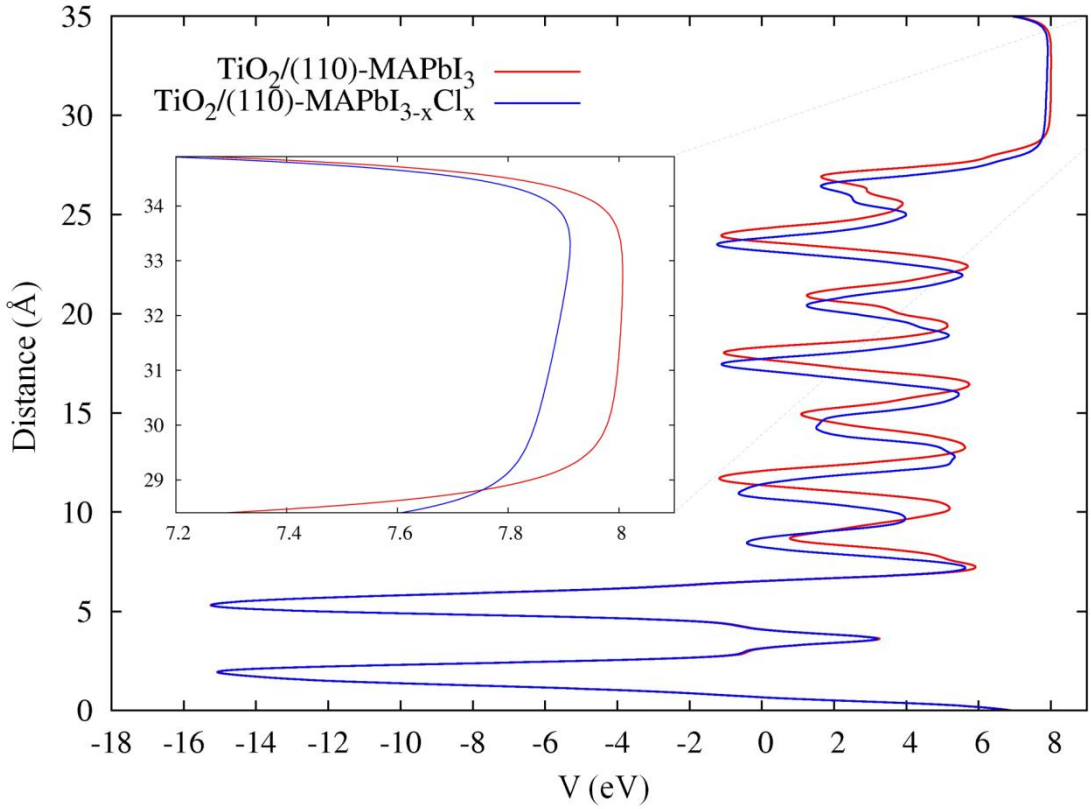

Figure S2. Integrated electrostatic potential along the direction normal to the TiO_2 surface. The inset shows a zoom of the vacuum region, where a bending of the electrostatic potential is calculated for the $MAPbI_{3-x}Cl_x$ perovskite, as opposed to the almost flat potential calculated for $MAPbI_3$.