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Supplementary information: Screening of Point Defects in Methylammonium Lead Halides: a Monte Carlo Study

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Additional MC data

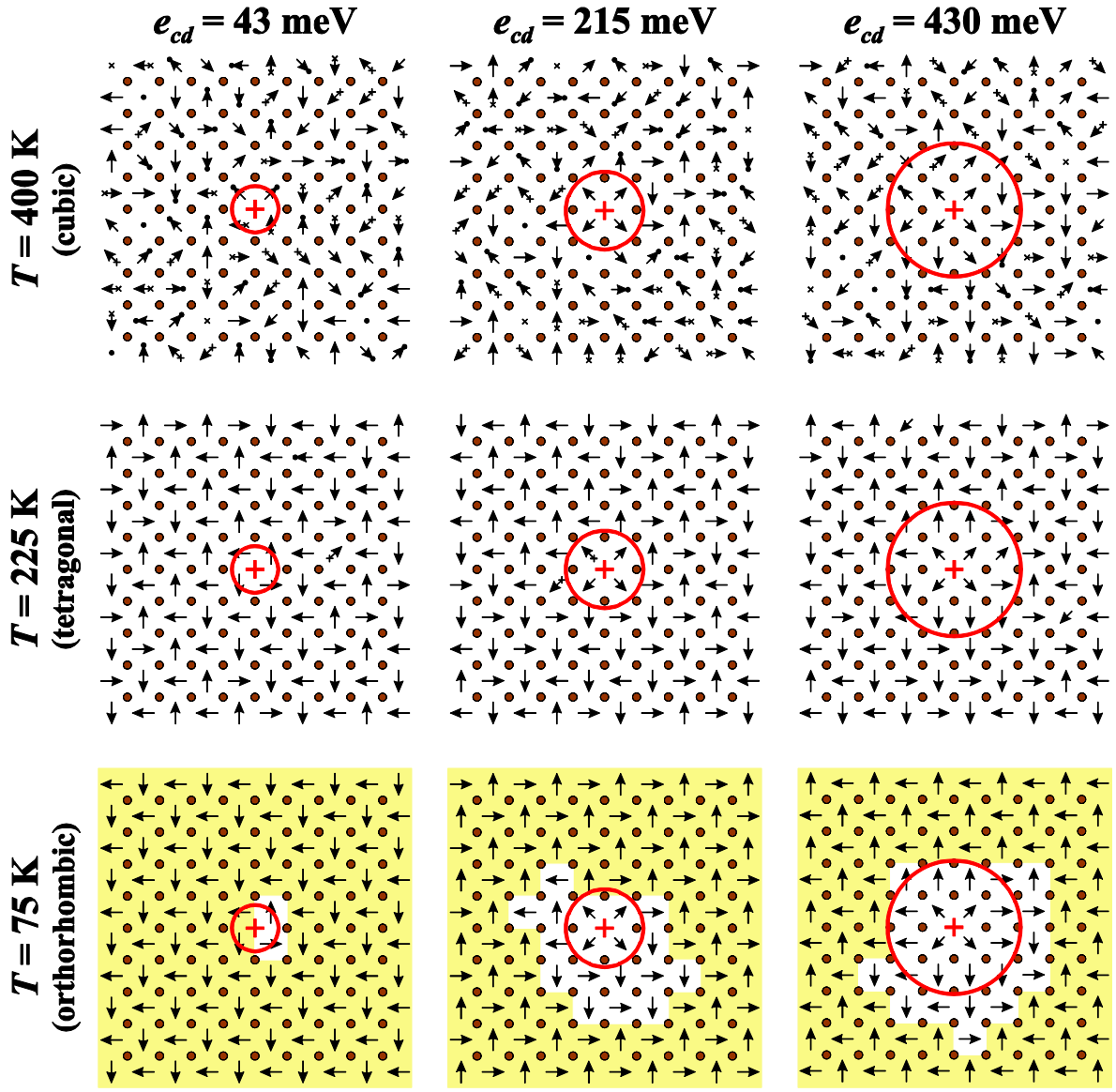

Figure S1. Arrangement of the MA^+ cations (black arrows) around a single positive halogen defect in the *ab*-plane obtained at different temperatures and e_{cd} interaction energies. The halogen atoms are represented as brown spheres. Temperatures correspond to the cubic, tetragonal and orthorhombic phases of $MAPbI_3$. The undisturbed long-range order of the MA^+ cations at 75 K is shaded in yellow. The red circles around the defects mark the apparent screening radius. Other simulation parameters: $e_1 = -43$, $e_2 = -21$, $e_{dd} = 8.6$ meV and $r_c = 10$.

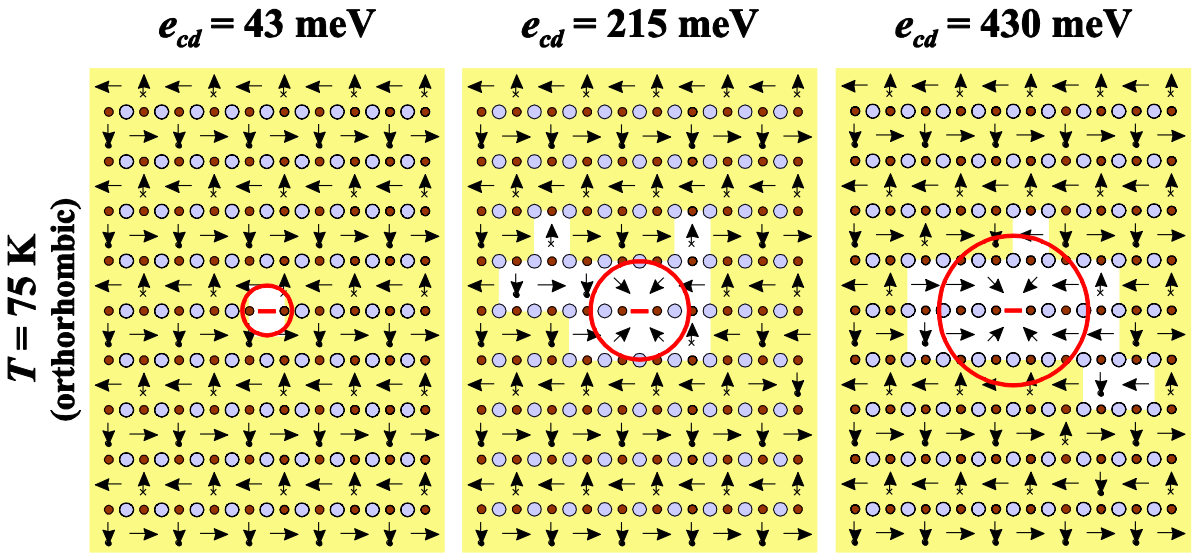

Figure S2. Arrangement of the MA^+ cations (black arrows) around a single negative Pb defect in the (011)-plane obtained at different temperatures and e_{cd} interaction energies. The halogen atoms are represented as brown spheres, while Pb atoms are gray. Temperatures correspond to the cubic, tetragonal and orthorhombic phases of $MAPbI_3$. The undisturbed long-range order of the MA^+ cations at 75 K is shaded in yellow. The red circles around the defects mark the apparent screening radius. Other simulation parameters: $e_1 = -43$, $e_2 = -21$, $e_{dd} = 8.6$ meV and $r_c = 10$.