Supporting Information

Unraveling the Water Degradation Mechanism of $CH_3NH_3PbI_3$

Chao Zheng* and Oleg Rubel *

Department of Materials Science and Engineering, McMaster University,

1280 Main Street West, Hamilton, Ontario L8S 4L8, Canada

The free energy surface of MA^+ dissolution in water is plotted in FIG. S1. This free energy surface is only for initial basin. It is obtained via ~4.7 ps metadynamics with a Gaussian height of 0.026 and a Gaussian weight of 0.014 and a continuous ~4.6 ps metadynamic calculation with a Gaussian height of 0.052 and a Gaussian weight of 0.018. We found the case of MA^+ calculation took much longer time staying at the initial basin. Due to the capability of our facility and limited time, we stopped for exploring the sequent free energy surface of MA^+ dissolution in water.

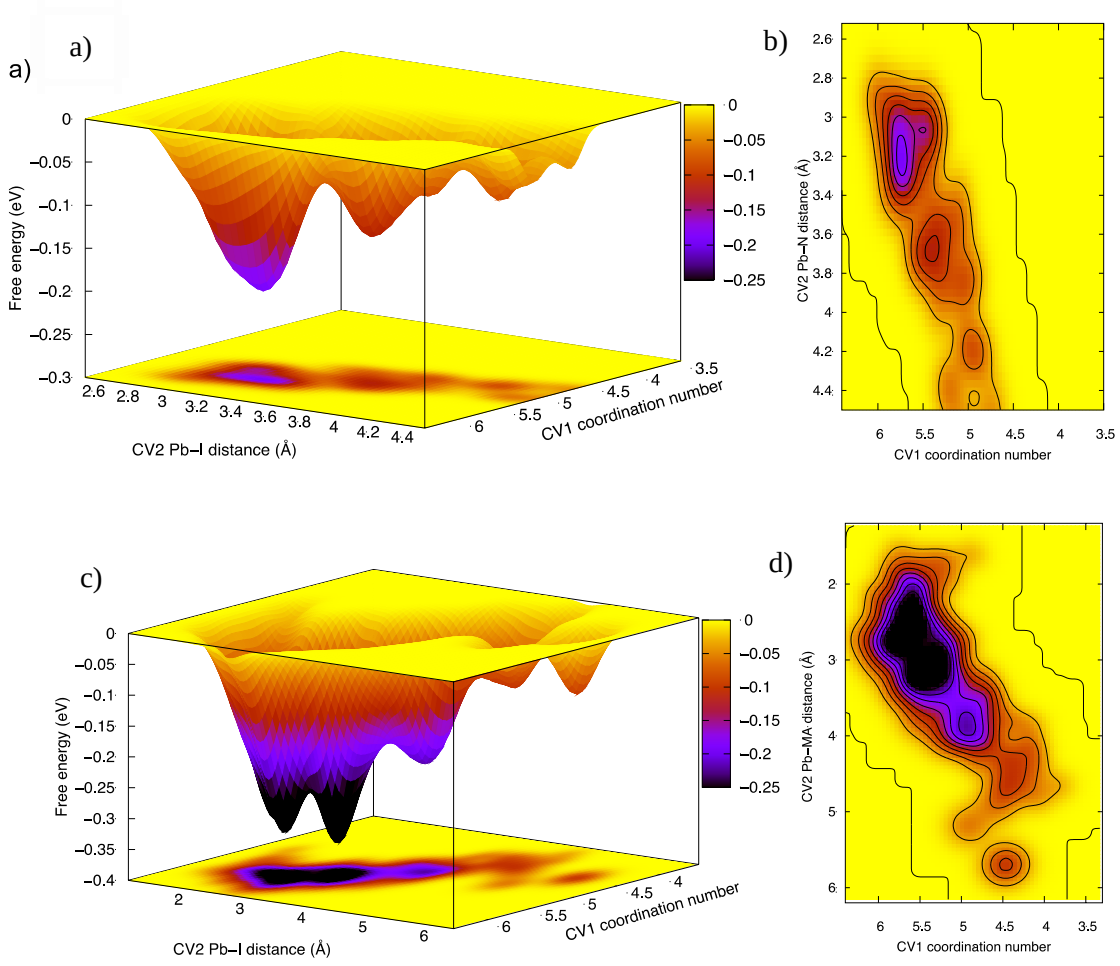

FIG. S1. (a) Free energy surface of initial basin of I^- dissolution in water. (b) Contour of the free energy surface of I^- dissolution in water. (c) Free energy surface of initial basin of MA^+ dissolution in water. (d) Contour of the free energy surface of MA^+ dissolution in water.

Comparing FIG. S1(a) and FIG. S1(c), we found the initial basin of MA^+ dissolution in water is deeper (~0.15 eV lower) than the value of I^- dissolution in water. And from FIG. S1(b) and FIG. S1(d), we found the initial basin of MA^+ dissolution in water is wider than the case of I^- dissolution in water. Hence, it explains the slow exploring rate and the inferiority of MA^+ dissolution in water for metadynamics.