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

Quantum Mechanical Molecular Dynamics Simulations of Polaron Formation in Methylammonium Lead Iodide Perovskite

Hiroki Uratani,[†] Chien-Pin Chou,[‡] and Hiromi Nakai[*,†,‡,¶]

†*Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, 3-4-1, Okubo, Shinjuku-ku, Tokyo 169-8555, Japan*

‡*Waseda Research Institute for Science and Engineering (WISE), 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan*

¶*Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Katsura, Kyoto 615-8245, Japan*

E-mail: nakai@waseda.jp

Table S1: Electronic parameters for Pb (in atomic units).

orbital type	W	a	r_0
s	6.76254	5.60847	4.54346
p	5.33981	9.14422	4.42425
d	4.58160	5.96026	4.80418
f	2.40562	2.83573	5.82248
density	7.01658	5.55764	4.23132

Table S2: Pb–I repulsive potential parameters (in atomic units).

a_1	a_2	a_3
2.067509E+00	5.616456E+00	-7.032404E-03

R_0	c_0	c_1	c_2	c_3	c_4
4.300000	3.082860992619E-02	-7.827799356081E-02	8.092023408549E-02	-3.003160069907E-02	5.128927793232E-05
4.609800	1.345202267925E-02	-3.678065883753E-02	5.303839964651E-02	-2.996804302586E-02	2.414304304420E-03
4.826300	7.676232444769E-03	-1.793104068906E-02	3.425313895081E-02	-2.787725549823E-02	1.727706606781E-04
4.831400	7.585671363570E-03	-1.758383384233E-02	3.382664390428E-02	-2.787373097675E-02	7.729573645229E-03
5.622500	4.072295874378E-03	-1.089048277048E-03	-3.301260240250E-03	-3.414268133792E-03	7.967429589431E-03
5.898700	3.494087064850E-03	-3.022546521069E-03	-2.483481779939E-03	5.388148076612E-03	-4.197780308028E-03
6.171900	2.569449999077E-03	-3.515425857717E-03	5.275477906474E-05	8.008137559991E-04	7.202015661719E-04
6.572200	1.240538476683E-03	-2.903436228347E-03	1.706883001333E-03	1.954000503753E-03	-3.804023645709E-03
6.778900	7.236369074490E-04	-2.081734329285E-03	1.943399762789E-03	-1.191166246519E-03	9.471375980340E-04
7.166000	1.611817555858E-04	-8.928732587616E-04	1.411649413755E-03	2.753816102771E-04	-1.765618955388E-03
*7.431500	2.001209625241E-05	-2.172276391035E-04	8.842373369206E-04	-1.599705720345E-03	1.085282035512E-03

*The last distance range ends at 7.800000 a.u..