

Supplementary Information for

BaTa_{0.5}Li_{0.5}O_{2.5}: A New Highly Oxygen Deficient Perovskite Oxide-Ion

Conductor

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(1) MSD data from AIMD simulations

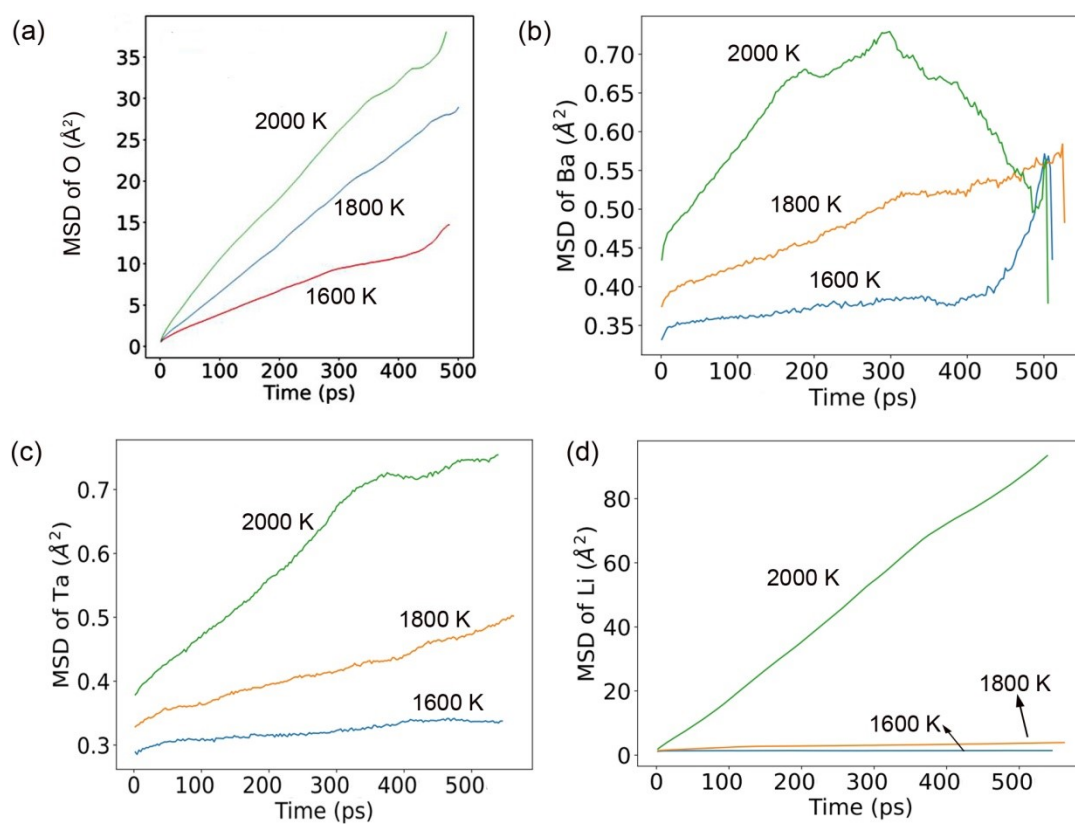


Figure S1. Mean square displacement (MSD) plot of (a) O^{2-} , (b) Ba^{2+} , (c) Ta^{5+} , and (d) Li^+ ions during AIMD simulations of three selected temperatures.