Supplementary Information (SI) for Physical Chemistry Chemical Physics.

First-principles molecular dynamics study on the behaviors of Cs in the mixed system of liquid metal and LiCl-KCl molten salt

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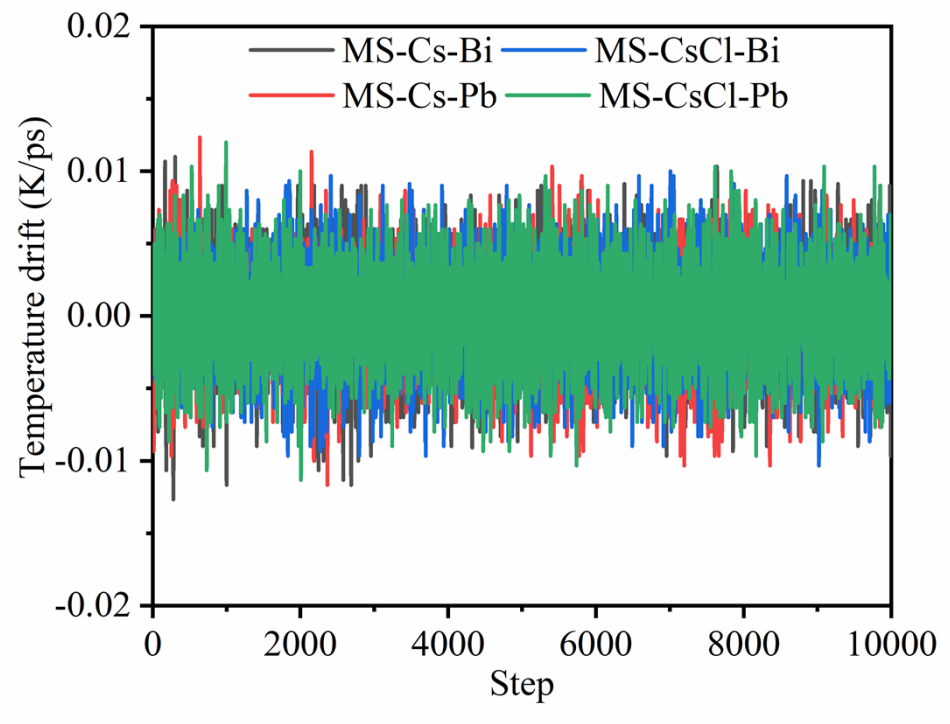

Figure S1. The temperature drift of the four systems during simulation process.

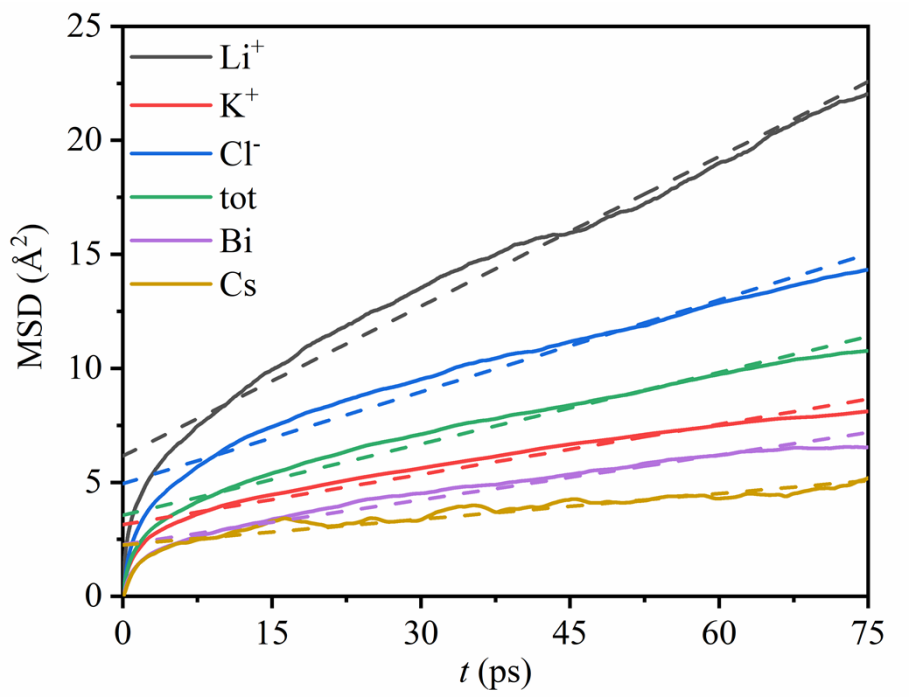

Figure S2. The MSD of each element in MS-Cs-Bi system for 75 ps. The dashed line is a linear fit.