Potential Energy Surfaces (PESs) of Ion-Model Compounds

This file contains potential energy surfaces (PES) of the ion-model compounds analyzed in the manuscript titled *"Balancing Group 1 Monoatomic Ion-Polar Compound Interactions in the Polarizable Drude Force Field: Applications in Protein and Nucleic Acid Systems."*

The dotted lines represent quantum mechanical (QM) results obtained using MP2/cc-pVQZ-X2C model chemistry for K^+, Rb^+, and Cs^+, and MP2/cc-pVQZ model chemistry for all other elements. Green and pink lines correspond to the molecular mechanical (MM) PESs from the original and new parameters, respectively. The cost function values are annotated and color-coded in each subplot, indicating the optimization performance of the force field parameters against the QM reference.