

Supplementary Information for “Representation of the QM Subsystem for Long-Range Electrostatic Interaction in Non-Periodic Ab Initio QM/MM Calculations”

Section S1. ANIONIC QM SUBSYSTEM: OLU⁻

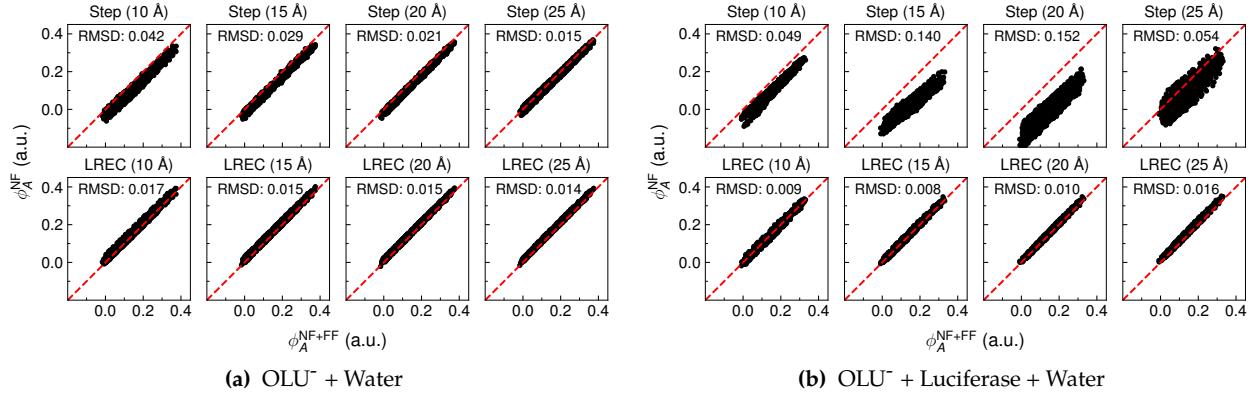


Figure S1. Atom-site potential from near-field MM charges *versus* atom-site potential from all MM charges. Each panel correspond to a different cutoff distance and either Step (near-field MM charges are not scaled) or LREC (near-field MM charges are scaled) scheme.

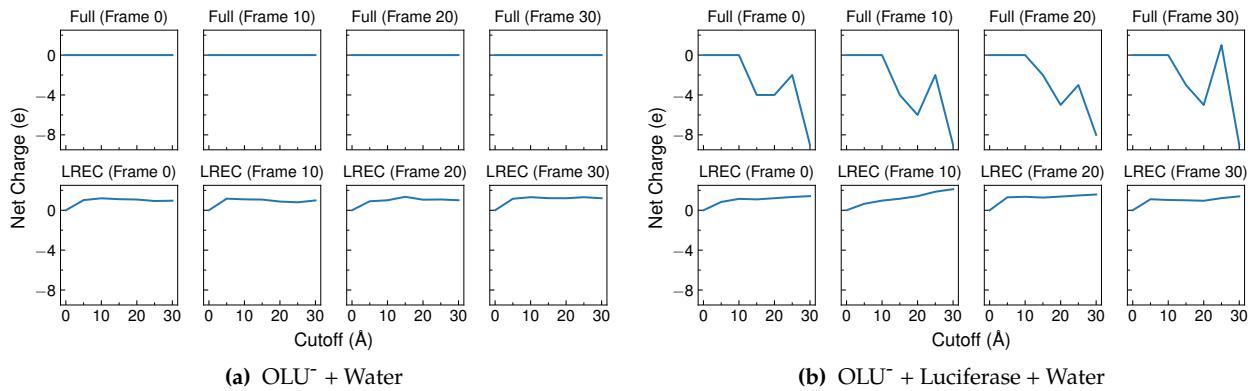


Figure S2. Sum of near-field MM charges at different cutoff distances. Each panel refers to either Step (near-field MM charges are not scaled) or LREC (near-field MM charges are scaled) scheme.