Constructing Simple yet Accurate Potentials for Describing the Solvation of HCl/Water Clusters in Bulk Helium and Nanodroplets - SUPPLEMENTARY MATERIAL -

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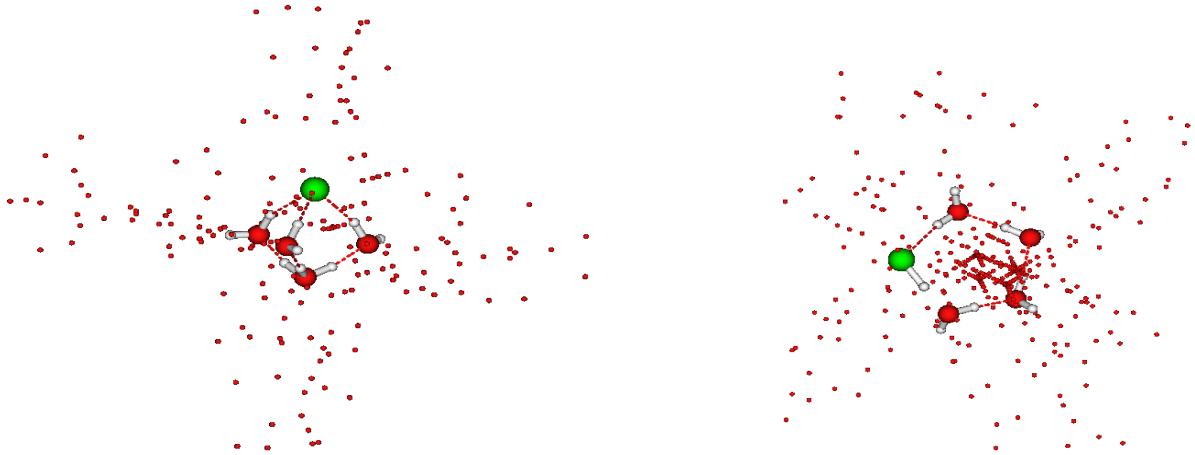

Figure S1: Small (l.h.s) and large (r.h.s.) grids of helium site positions for two different cluster structures.

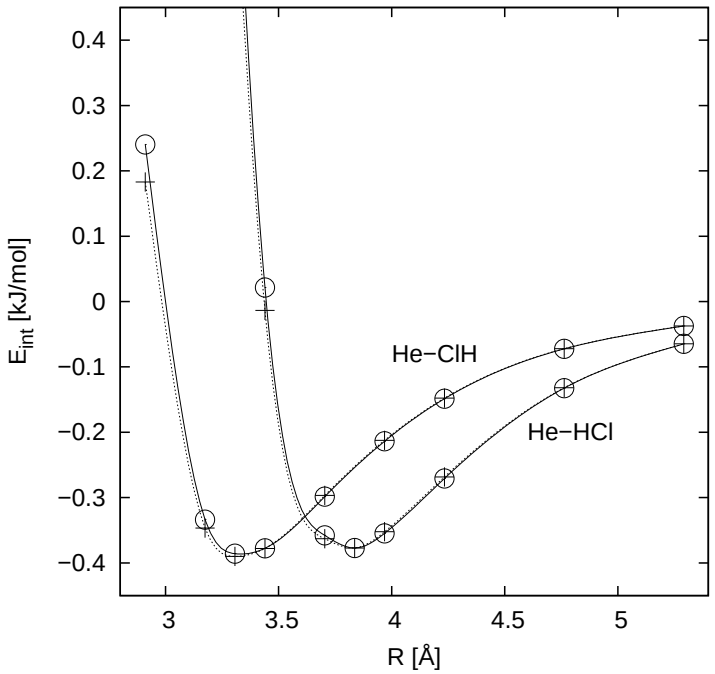

Figure S2: Potential energy curves for the linear orientations of He···HCl. Circles: CCSD(T)/cbs(Q5) interaction energies; crosses: DFT-SAPT/cbs(TQ).

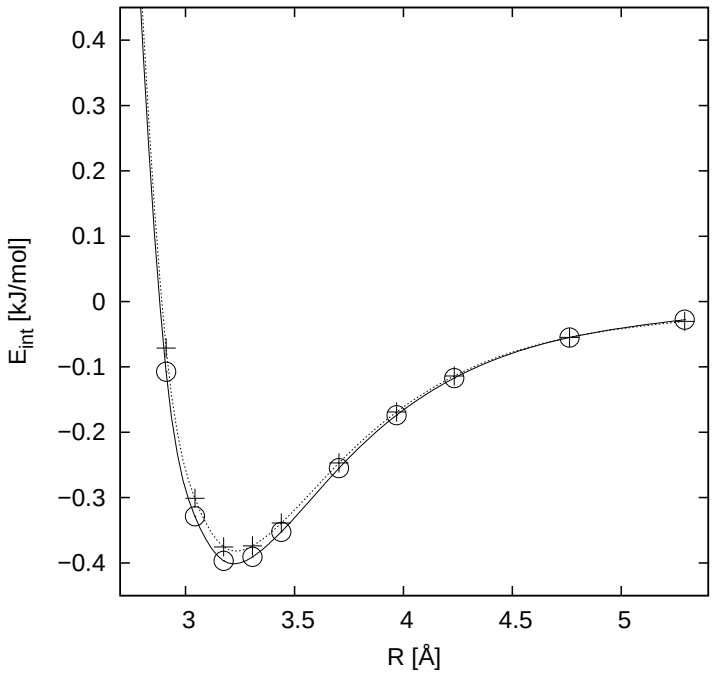

Figure S3: Potential energy curve for the planar rectangular orientation of $He\cdots H_2O$. Circles: CCSD(T)/cbs(Q5) interaction energies; crosses: DFT-SAPT/cbs(TQ).

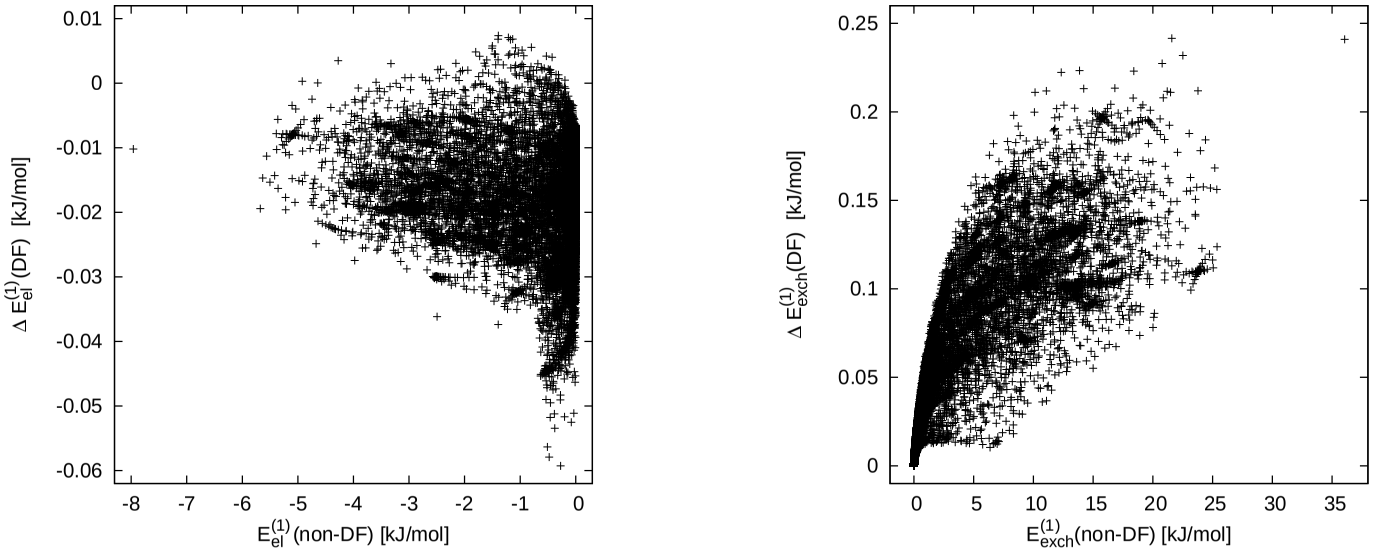

Figure S4: HF-SAPT/aVDZ density fitting errors $\Delta E^{(1)} = E^{(1)}(\mathrm{DF}) - E^{(1)}(\mathrm{non-DF})$ at the small helium grid positions around $HCl(H_2O)_4$.

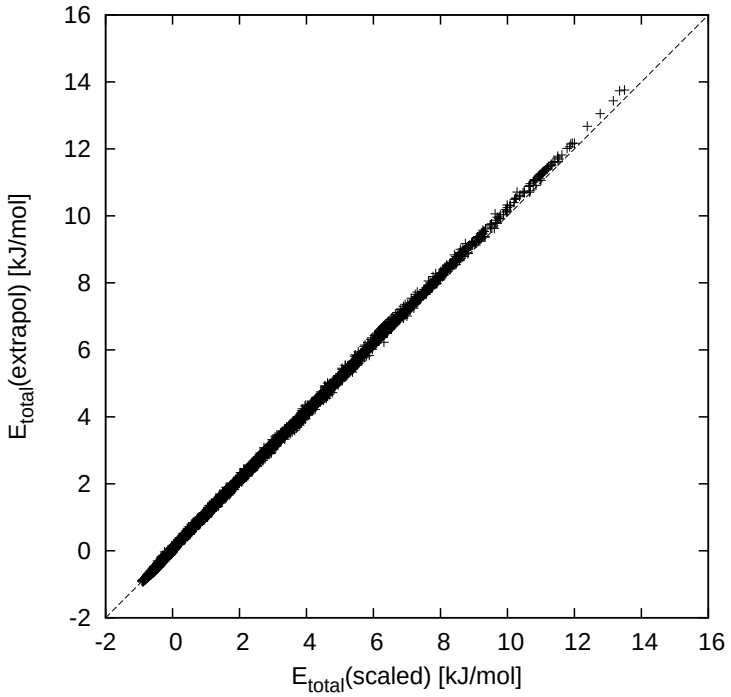

Figure S5: DFT-SAPT interaction energies with scaled DZ dispersion contribution compared to interaction energies with DZ/TZ-extrapolated dispersion contributions.

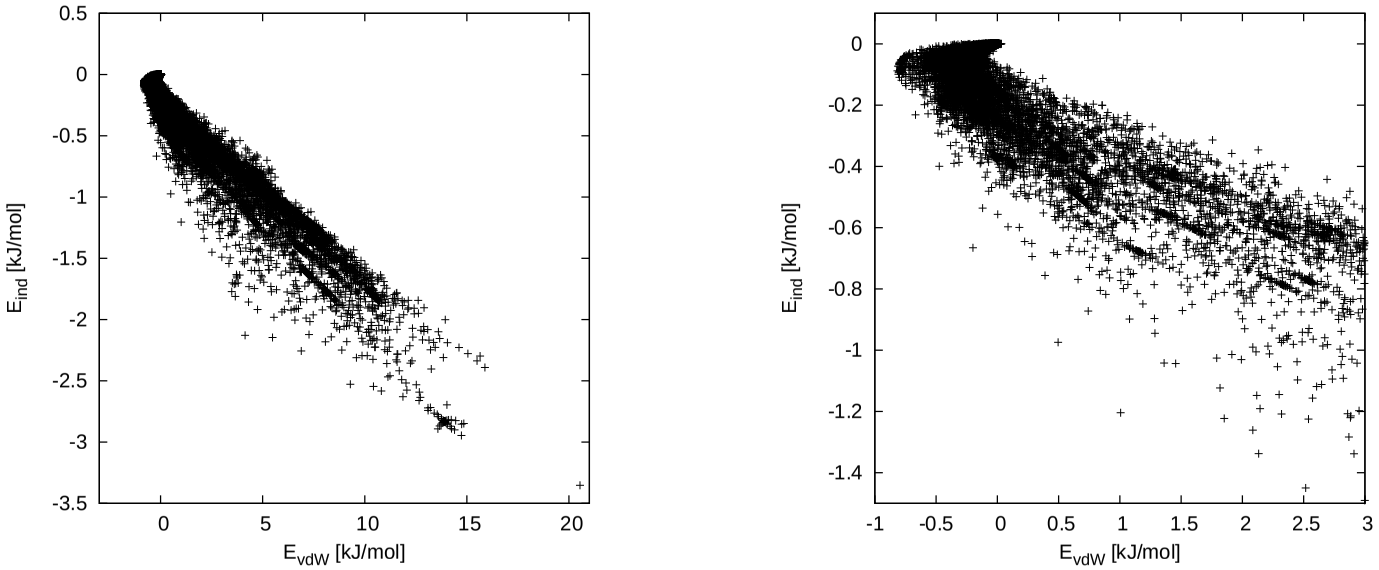

Figure S6: Van der Waals-energies compared to induction energies.

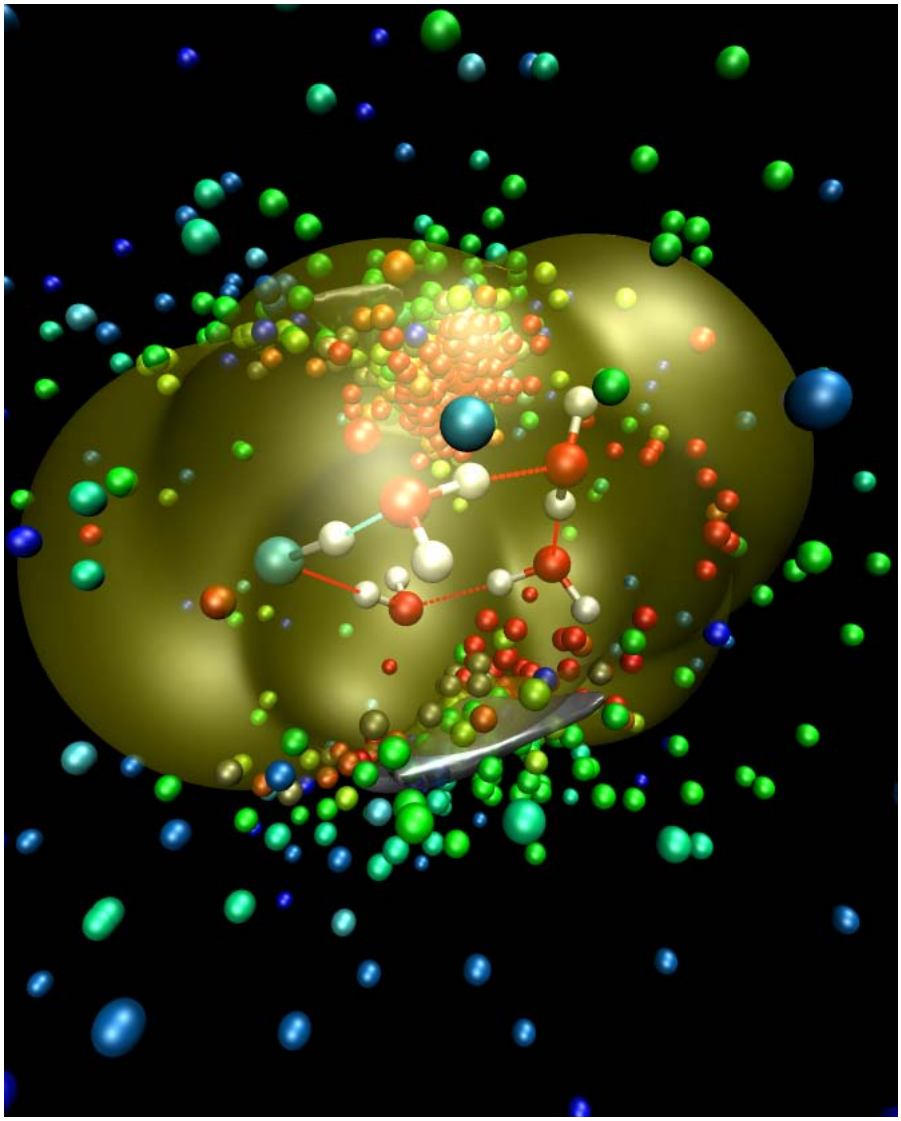

Figure S7: Detailed comparison of fitted model potential vs. reference values for the undissociated (UD) cluster structure. The color coding is the same as in Fig. 1 of the main text.

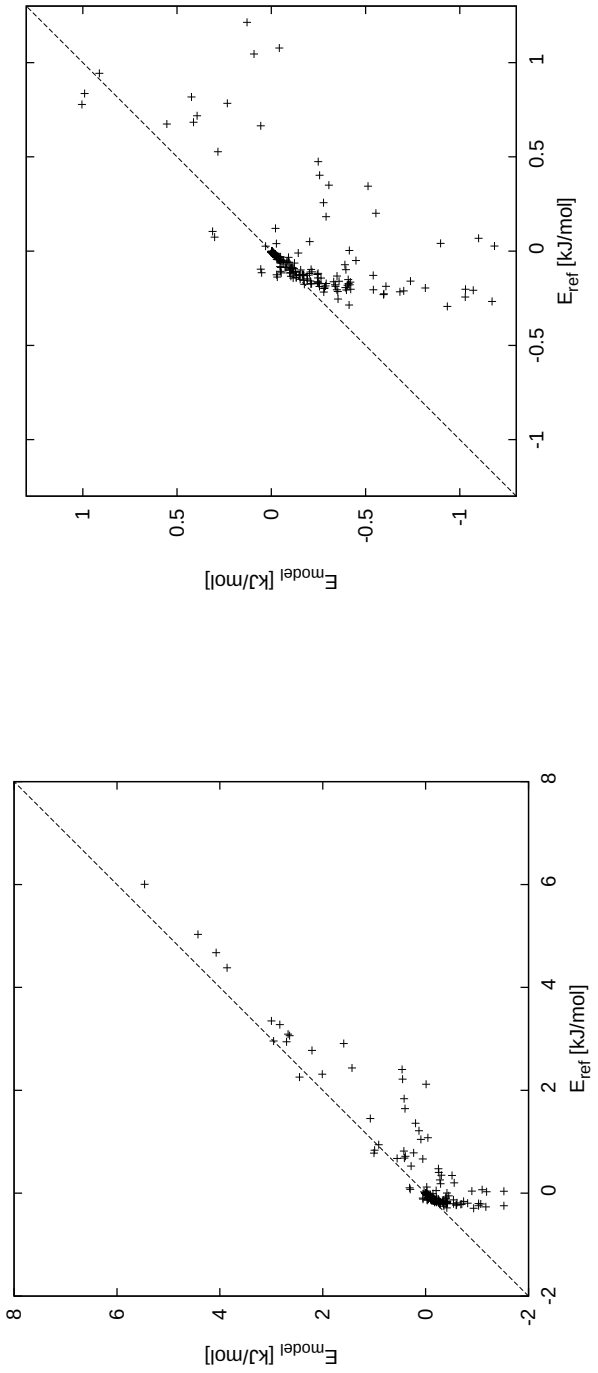

Figure S8: Comparison of fitted model potential vs. reference values for water.

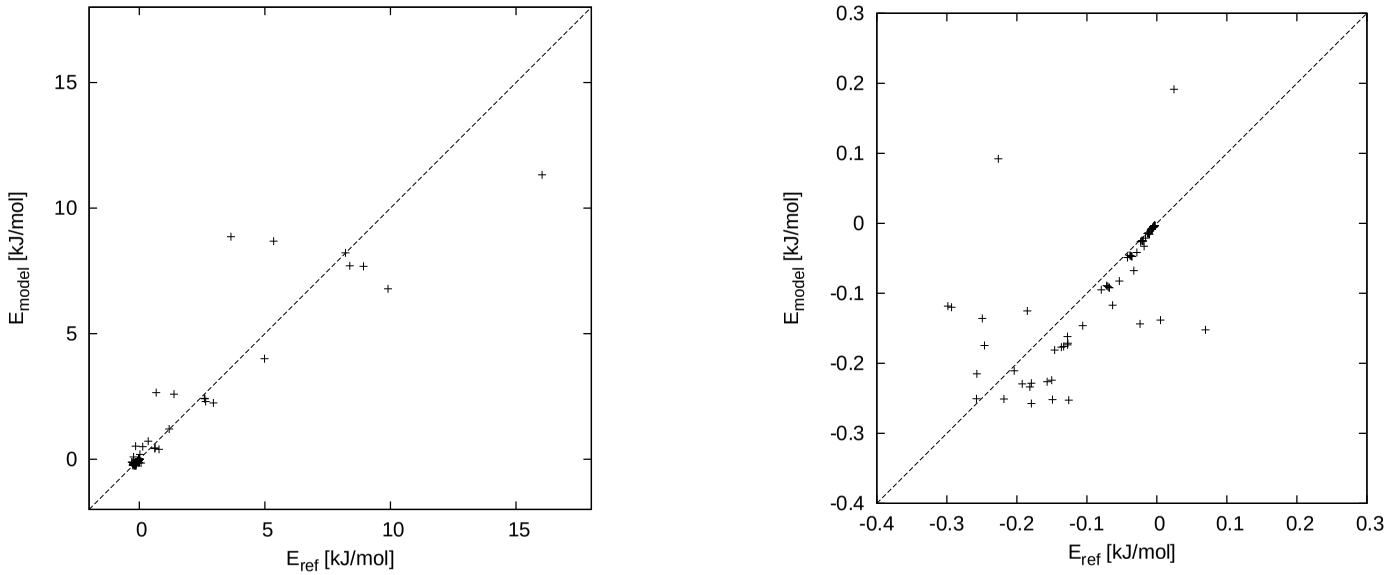

Figure S9: Comparison of fitted model potential vs. reference values for hydrogenchloride.