I. DETAILED MODEL POTENTIAL

TABLE I: Detailed Model Parameters

Symbol	Value	Source / Description
R_{OH}	0.9572Å	Gas-phase geometry
$\widehat{\mathrm{HOH}}$	104.52°	
$\mathrm{q_H}$	0.605 e	Gas-phase charge moments
R_{OM}	0.2667Å	
ω	0.6287 $E_h/\hbar$	Gas-phase polarization and dispersion responses
m	0.3656 m_e	
q_d	-1.1973 e	
σ_d	0.1 a_0	Gaussian charge widths for drudon, tether-point (center), H-atom and M-site - damp Coulomb force at short range
σ_c	1.2 a_0	
σ_{H}	0.1 a_0	
σ_{M}	0.1 a_0	
κ_1	2.5 E_h	O-O repulsion parameters
λ_1	1.171802 a_0^{-1}	
κ_2	6000 E_h	
λ_2	2.820276 a_0^{-1}	

A. Coulomb potential with Gaussian charge width

For a Gaussian distribution with width σ, the enclosed volume as a function of radius is the error function:

$$\begin{aligned} \rho(r) &= q\tfrac{1}{\sqrt{2\pi}\sigma}\exp\left(-\tfrac{r^2}{2\sigma^2}\right), \\ \nabla^2\phi &= \rho \implies \\ \phi(r) &= \frac{q\,\mathrm{erf}(r/\sqrt{2}\,\sigma)}{r}. \end{aligned}$$

For two Gaussian distributions interacting, we can use the fact that variances of independent variables add:

$$\begin{aligned} \sigma_{12}^2 &\to \sigma_1^2 + \sigma_2^2, \\ \phi(r) &= \frac{q_1 q_2\,\mathrm{erf}(r/\sqrt{2}\,\sigma_{12})}{r}. \end{aligned}$$

B. Exponential repulsive potential

This model adds a repulsion potential between the O-atoms, with two exponential terms:

$$\phi(r) = \kappa_1\exp(-\lambda_1 r) + \kappa_2\exp(-\lambda_2 r).$$

Note that κ_i and λ_i are not related to the dispersion scaling parameter κ nor the polarizability scaling parameter λ mentioned in the text.