

Supporting Information

Water desalination of a new three-dimensional covalent organic framework: a molecular dynamics simulation study

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The accuracy through comparing simulation results employing CVFF, COMPASS and UFF forcefields was checked. The force field of Condensed-Phase Optimized Molecular Potential for Atomistic Simulation Studies (COMPASS) was used to consider interatomic interaction [1]. COMPASS, a widely used all-atom force field based on ab initio and optimized by experimental data, has been validated to be capable of accurately predicting structural and thermophysical properties for a broad range of organic and inorganic substances. The universal force field (UFF) is a broadly applicable classical force field that contains parameters for almost every atom type of the periodic table [2, 3]. Such a flexibility makes UFF applicable to a broad spectrum of systems, which has been demonstrated through evaluations on organic molecules [4], main group compounds [5], and metal-organic frameworks (MOFs) [6].

The interactions of COF atoms were modeled by the Lennard-Jones (LJ) and electrostatic potentials:

$$V_{\text{non-bonded}} = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \quad (1)$$

As to the LJ parameters, they were adopted from the CVFF, COMPASS and UFF, respectively. As to the atomic charges, in UFF forcefield, they were assigned using the Density-Derived Electrostatic and Chemical (DDEC) method [7-8] based on density functional theory calculations as described in the reference [9]. In COMPASS, the atomic charges were assigned automatically through the forcefield itself [10-12].

The nonbonded parameters (LJ parameters and atomic charge) determine the accuracy of MD results. Here, two simulation parameters which were closely determined by the LJ parameters and atomic charges were employed to prove the accuracy of nonbonded parameters. One is the interaction energy between the COF and water, the other is the radial distribution function of H₂O to COF.

The interaction energy the COF and water was calculated by equation (2),

$$E_{\text{COF/H}_2\text{O}} = E_{\text{COF}} + E_{\text{H}_2\text{O}} - E_{\text{COF+H}_2\text{O}} \quad (2)$$

Where $E_{\text{COF/H}_2\text{O}}$ is the interaction energy between COF and H₂O, $E_{\text{COF+H}_2\text{O}}$ is the total potential energy of COF and H₂O. E_{COF} and $E_{\text{H}_2\text{O}}$ represent the potential energy of COF and H₂O, respectively.

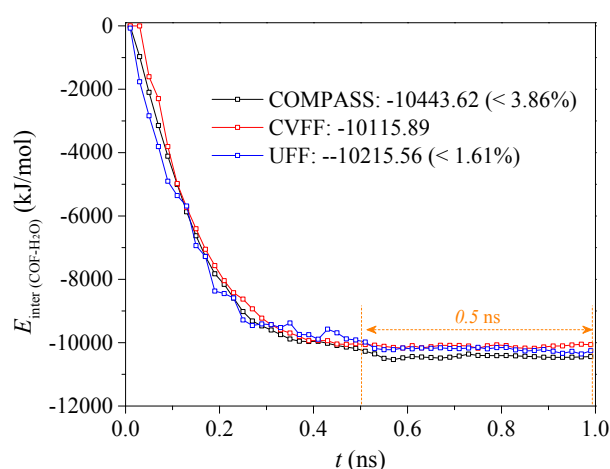


Figure S1. The interaction energy between the COF and H₂O molecules in the systems calculated employing COMPASS, CVFF and UFF forcefields. The average energy values corresponding to the last 0.5 ns were calculated.

Based on the data in the Figure S1, the interaction energy difference from CVFF are less than 3.86% and 1.61% in the systems with COMPASS and UFF, respectively. From the little difference of interaction energy, we can conclude that it is feasible to use CVFF forcefield to calculate the fixed COF.

Furthermore, the radial distribution functions (*RDFs*) profiles of H₂O-COF in three systems were calculated shown in Figure S2. The *RDFs* could be calculated by equation [13]:

$$g(r) = \rho_{(r)}/\rho_0 \quad (3)$$

where $\rho_{(r)}$ is the local number density, and ρ_0 is the bulk number density. The *RDFs* describes the probability of the particle B presents at the distance r from the targeted particle A.

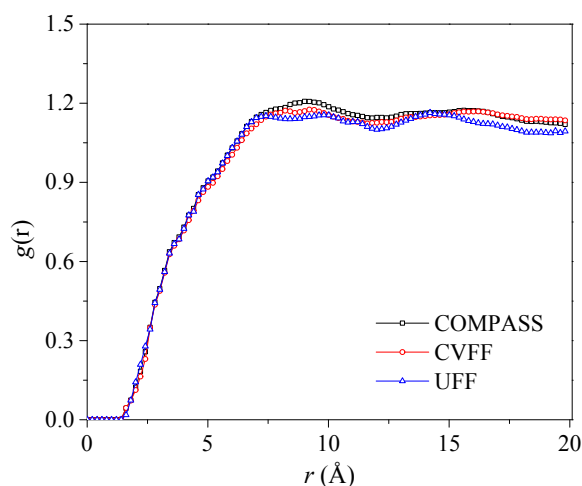


Figure S2. The radial distribution functions (*RDFs*) profiles of H₂O-COF in the systems with COMPASS, CVFF and UFF.

The spatial distribution characteristics of H₂O molecules as shown in Figure S2 is nearly consistent, indicating that the interaction between H₂O and COF in three forcefields is similar. Thus, the RDF results of H₂O-COF further confirms the rationality of the CVFF.

In conclusion, three universally used forcefields were employed to calculate interaction energy and RDF closely determined by the nonbonded parameters, the negligible difference indicates the nonbonded parameters obtained from CVFF forcefield is reliable.

Reference

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