Electronic Supplementary Material (ESI) for RSC Advances.

Interactions of Pt nanoparticle with molecular components in polymer electrolyte membrane fuel cells: Multi-scale modeling approach

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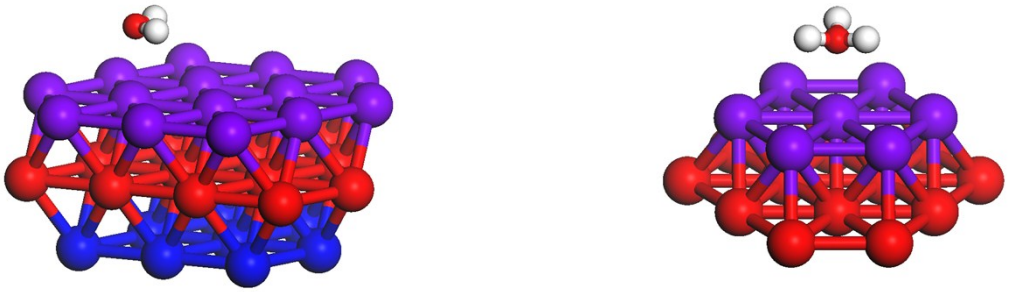
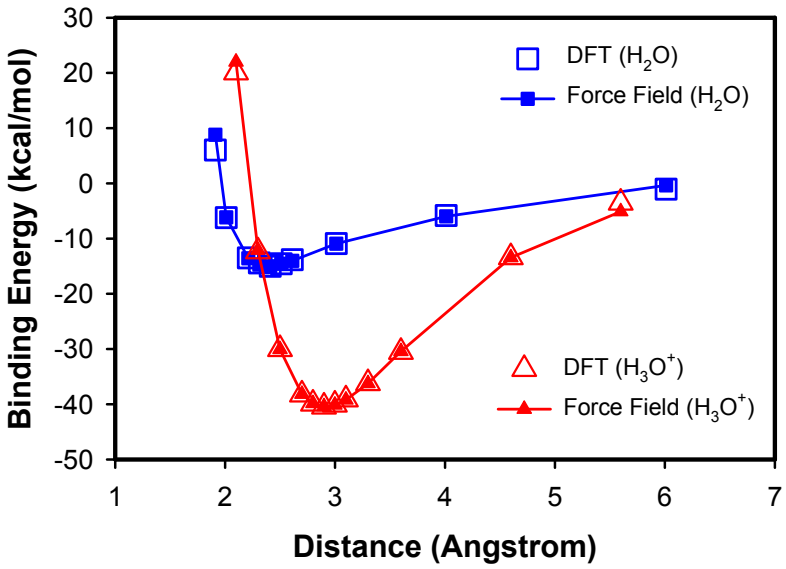


(a) (b)



(c)

Figure S1. Adsorptive binding energy of H_2O (water) and H_3O^+(hydronium) molecule on Pt (111) surface: (a) optimized geometry of H_2O-$Pt_{14\text{-}13\text{-}8}$; (b) optimized geometry of H_3O^+-$Pt_{12\text{-}7}$; (c) change of binding energy of H_2O and H_3O^+ on Pt (111) surface as a function of distance. For DFT calculations, M06 functional is used with LACVP** basis set. For force field calculations, Morse potential function is used with newly optimized off-diagonal van der Waals parameters.

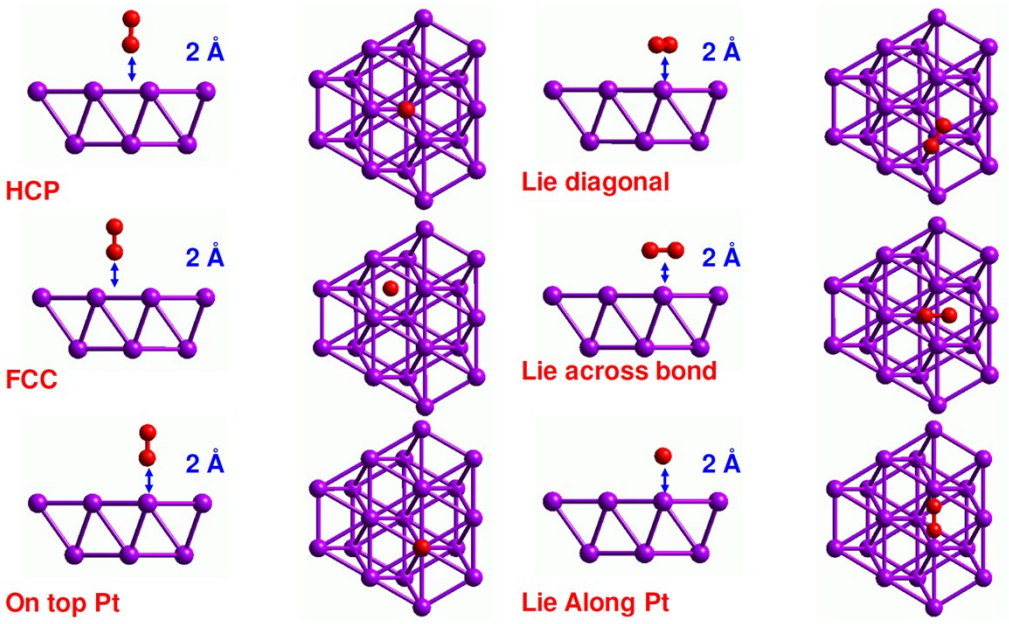
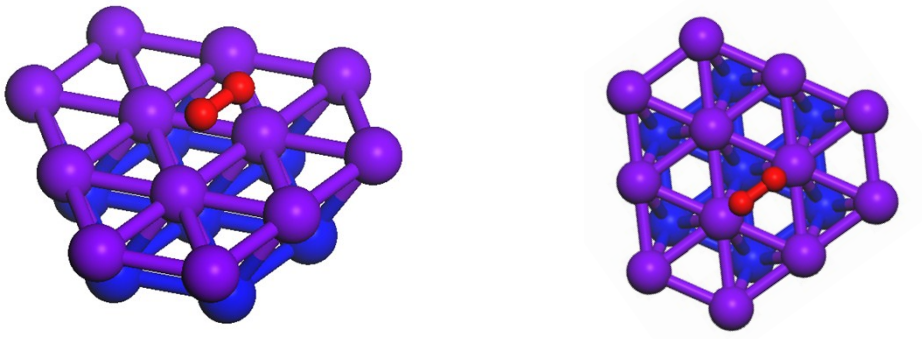
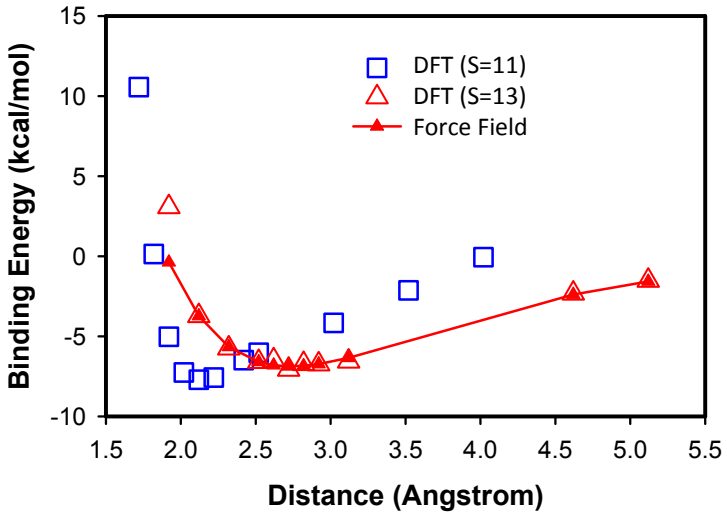


Figure S2. Side and top views of the six initial configurations before geometrically optimizing molecular oxygen on the Pt surface.



(a) (b)



(c)

Figure S3. Adsorptive binding energy of O_2 (oxygen) molecule on Pt (111) surface: (a) tile view of optimized geometry of O_2-$Pt_{14\text{-}13\text{-}8}$; (b) top view of optimized geometry; (c) change of binding energy of O_2 on Pt (111) surface as a function of distance. For DFT calculations, M06 functional is used with LACVP** basis set. For force field calculations, Morse potential function is used with newly optimized off-diagonal van der Waals parameters.

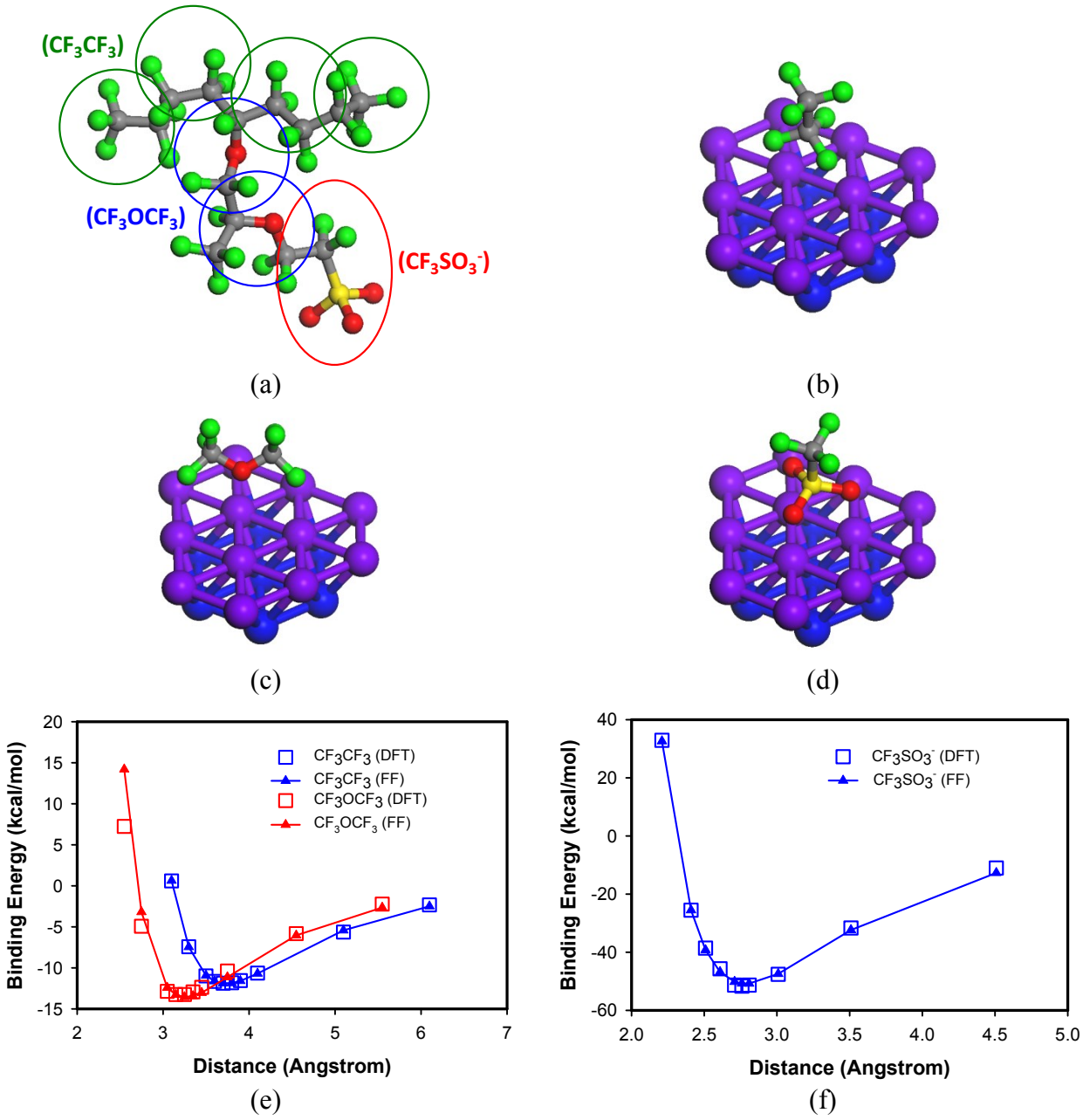
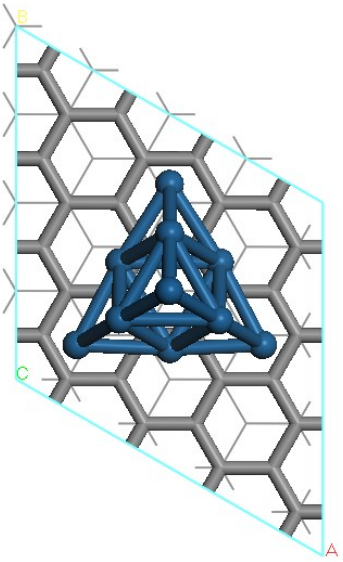
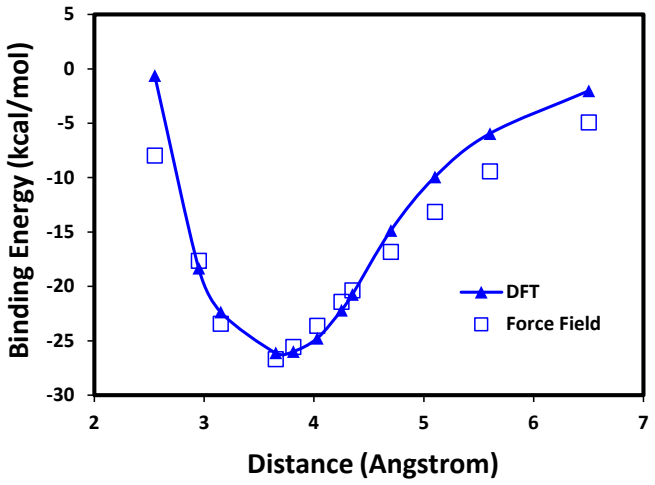


Figure S4. Adsorptive binding energy of fragments of polymer electrolyte (Nafion) on Pt (111) surface: (a) fragments of Nafion; (b) optimized geometry of CF_3CF_3-Pt_{12-7}; (c) optimized geometry of CF_3OCF_3-Pt_{12-7}; (d) optimized geometry of $CF_3SO_3^-$-Pt_{12-7}; (e) change of binding energy for CF_3CF_3-Pt_{12-7} and CF_3OCF_3-Pt_{12-7}; (f) change of binding energy for $CF_3SO_3^-$-Pt_{12-7}. For DFT calculations, M06 functional is used with LACVP** basis set. For force field calculations, Morse potential function is used with newly optimized off-diagonal van der Waals parameters.



(a)



(b)

Figure S5. Adsorptive binding energy of $Pt_{6\text{-}3\text{-}1}$ cluster model on graphite surface: (a) optimized structure of $Pt_{6\text{-}3\text{-}1}$ on graphite; (b) change of binding energy of $Pt_{6\text{-}3\text{-}1}$ on graphite surface as a function of distance. For DFT calculations, PBE-D3 functional is used with DNP basis set. For force field calculations, Morse potential function is used with newly optimized off-diagonal van der Waals parameters.