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

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Figure S1. Adsorptive binding energy of $\text{H}_2\text{O}$ (water) and $\text{H}_3\text{O}^+$ (hydronium) molecule on Pt (111) surface: (a) optimized geometry of $\text{H}_2\text{O}$-Pt$_{14-13-8}$; (b) optimized geometry of $\text{H}_3\text{O}^+$-Pt$_{12-7}$; (c) change of binding energy of $\text{H}_2\text{O}$ and $\text{H}_3\text{O}^+$ 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.
Figure S3. Adsorptive binding energy of O$_2$ (oxygen) molecule on Pt (111) surface: (a) tile view of optimized geometry of O$_2$-Pt$_{14-13-8}$; (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$_3$CF$_3$-Pt$_{12-7}$; (c) optimized geometry of CF$_3$OCF$_3$-Pt$_{12-7}$; (d) optimized geometry of CF$_3$SO$_3$-Pt$_{12-7}$; (e) change of binding energy for CF$_3$CF$_3$-Pt$_{12-7}$ and CF$_3$OCF$_3$-Pt$_{12-7}$; (f) change of binding energy for CF$_3$SO$_3$-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.
Figure S5. Adsorptive binding energy of Pt\(_{6-3-1}\) cluster model on graphite surface: (a) optimized structure of Pt\(_{6-3-1}\) on graphite; (b) change of binding energy of Pt\(_{6-3-1}\) 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.