Supporting Information

Mechanistic Insight into the Oxygen Reduction Reaction on Mn-N_4/C Single Atom Catalyst: The Role of the Solvent Environment

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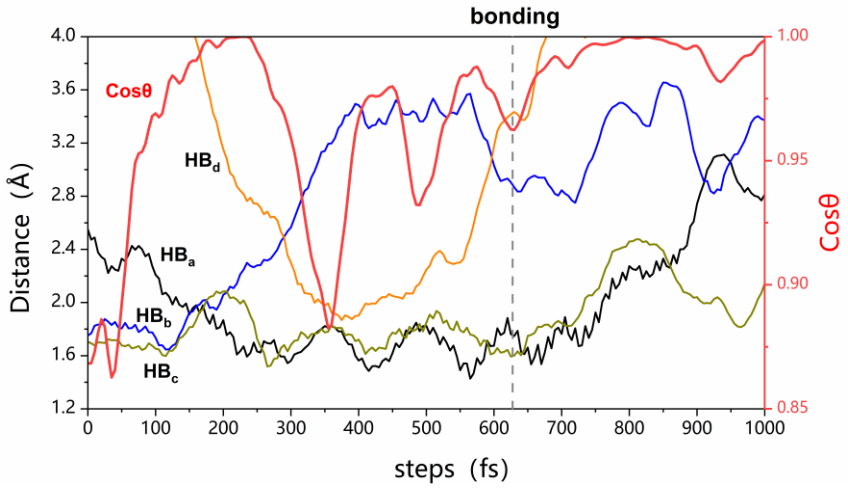

Figure S1. The evolution of bond lengths of hydrogen bonds (H_a, H_b, H_c, H_d) and Cosθ at the initial stage of AIMD simulations.

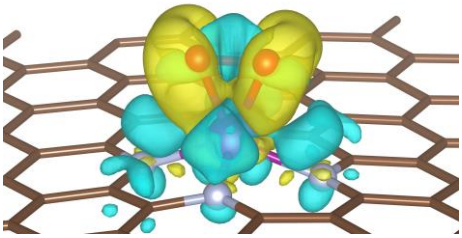

Figure S2. Charge density differences of "side-on" O_2 adsorption on GP model. Yellow area denotes the electron-density increase and blue area denotes the electron-density decrease.

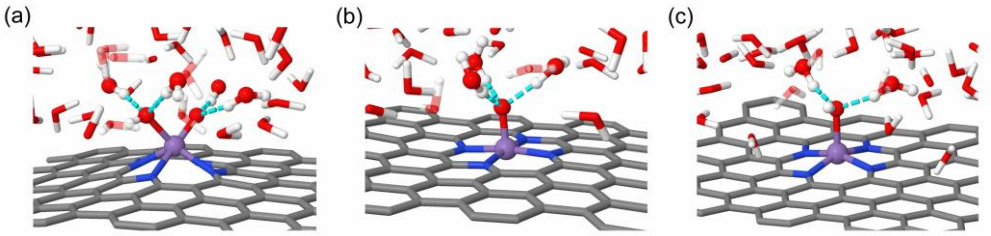

Figure S3. The stable configurations of reaction intermediates during ORR on LP model **(a)** O*OH, **(b)** *O, and **(c)** *OH. The green lines denote the formation of hydrogen bonds.