

Insights into the Adsorption of Oxygen and Water on Low-Index Pt Surfaces by Molecular Dynamics Simulations

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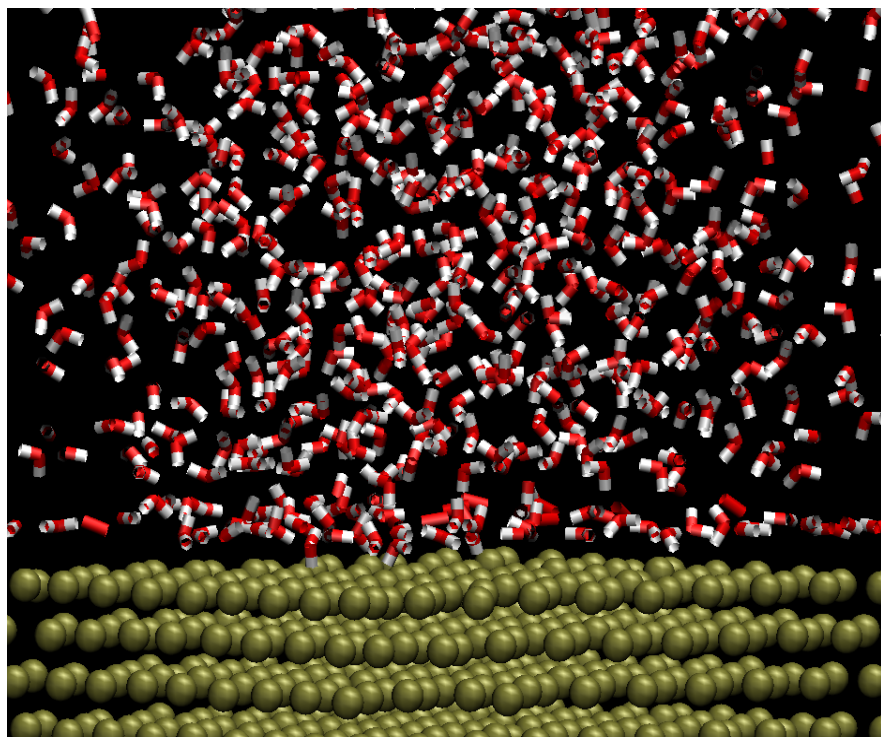
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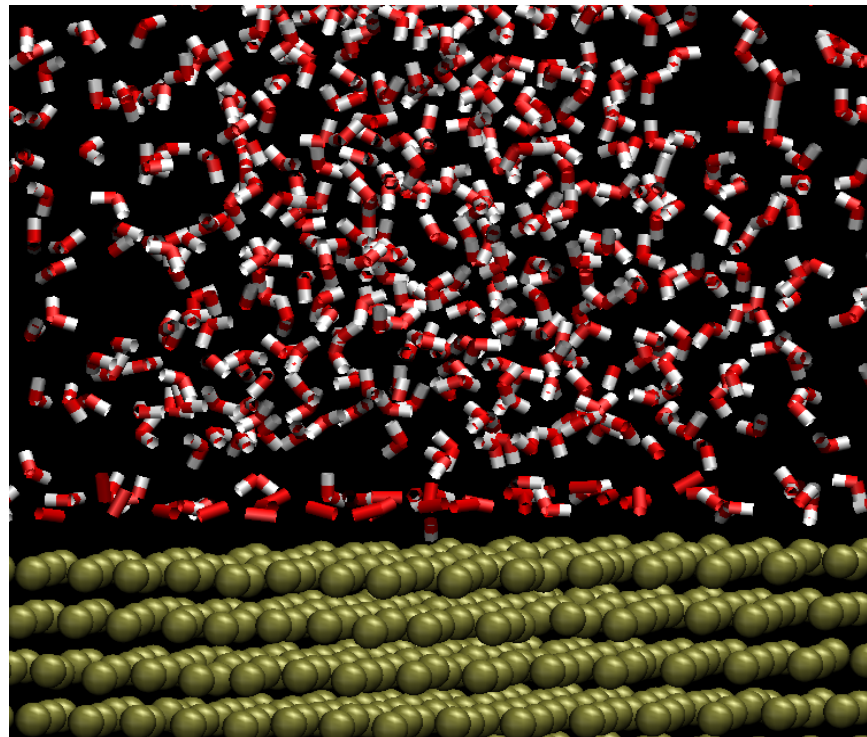
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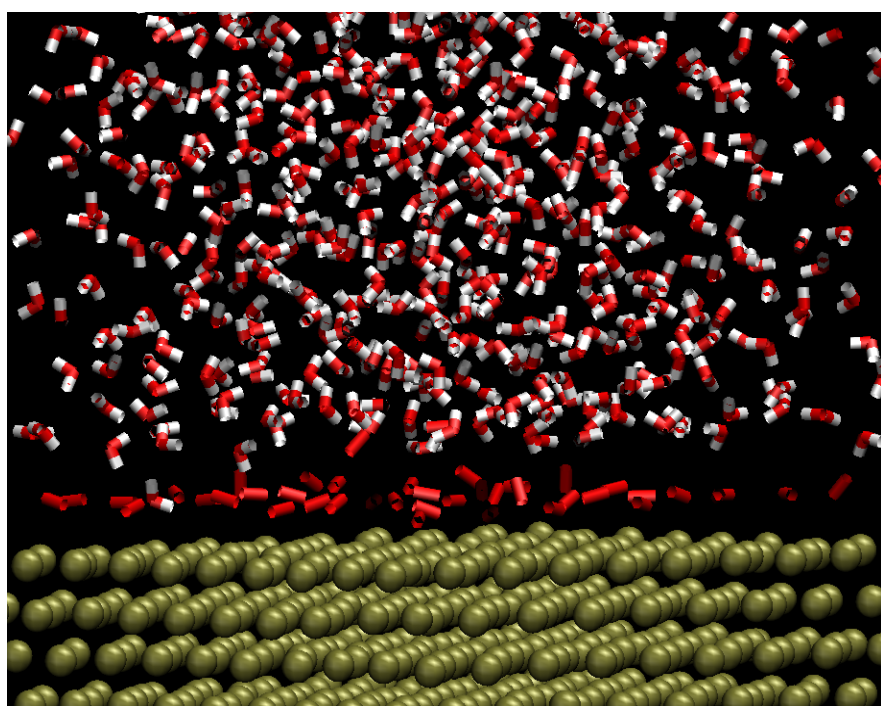
Supporting Information



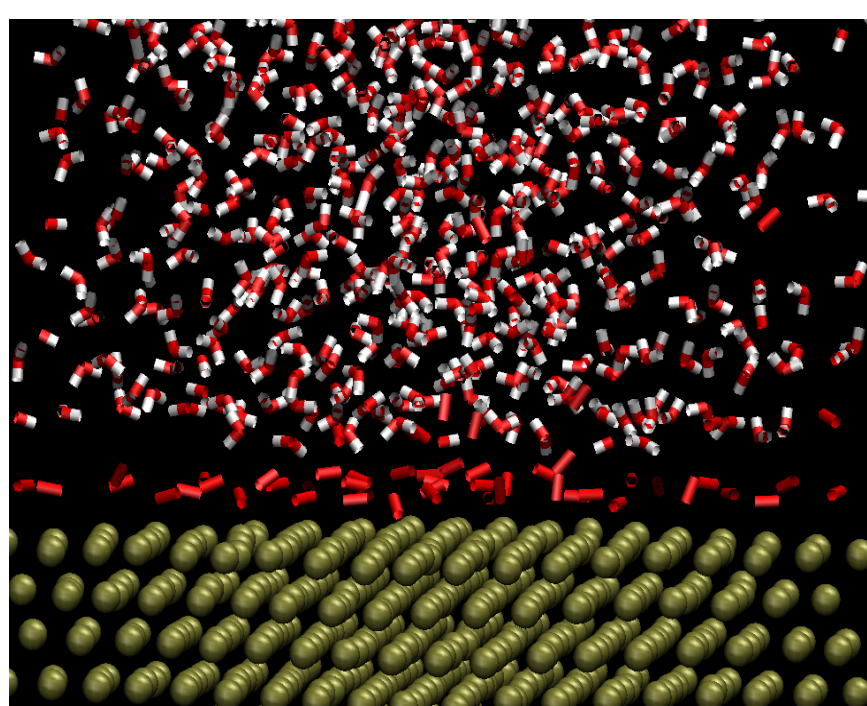
Pt (111)/16O₂/H₂O



Pt (111)/32O₂/H₂O

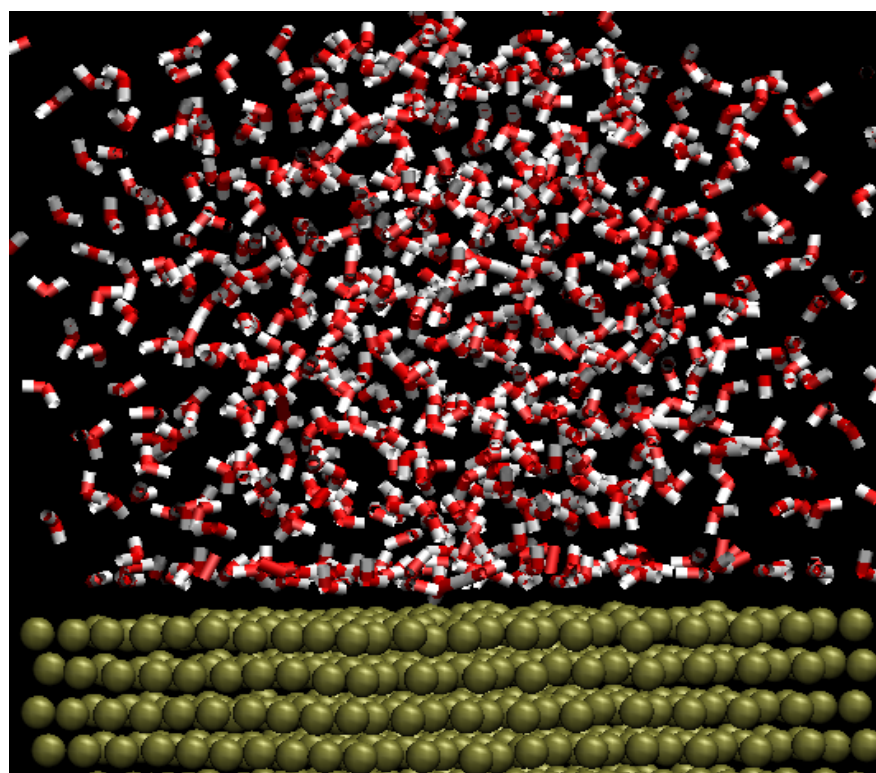


Pt (111)/48O₂/H₂O

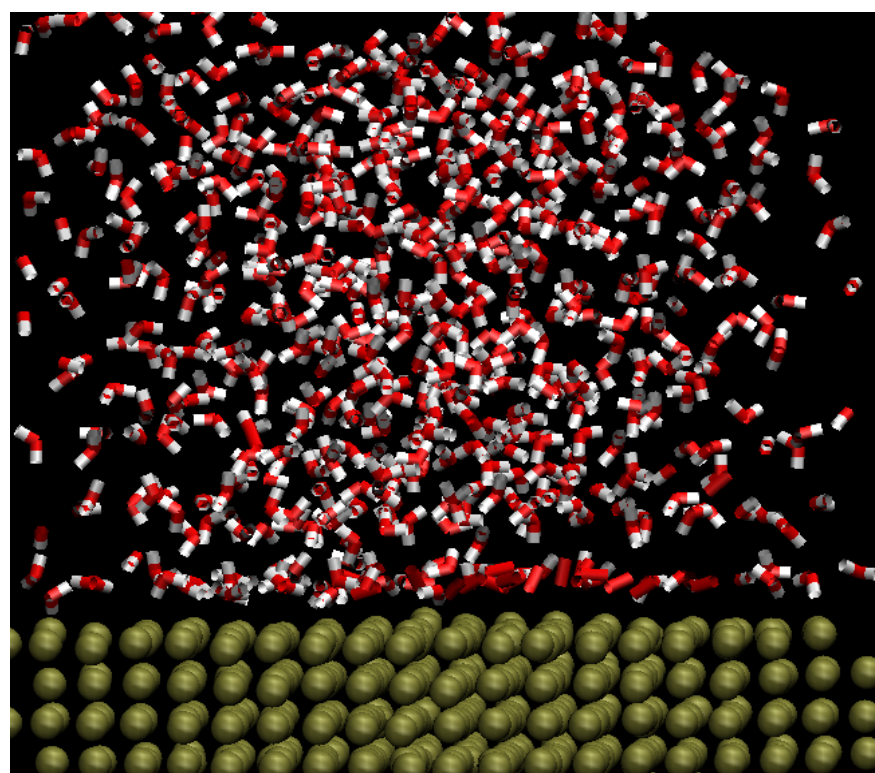


Pt (111)/64O₂/H₂O

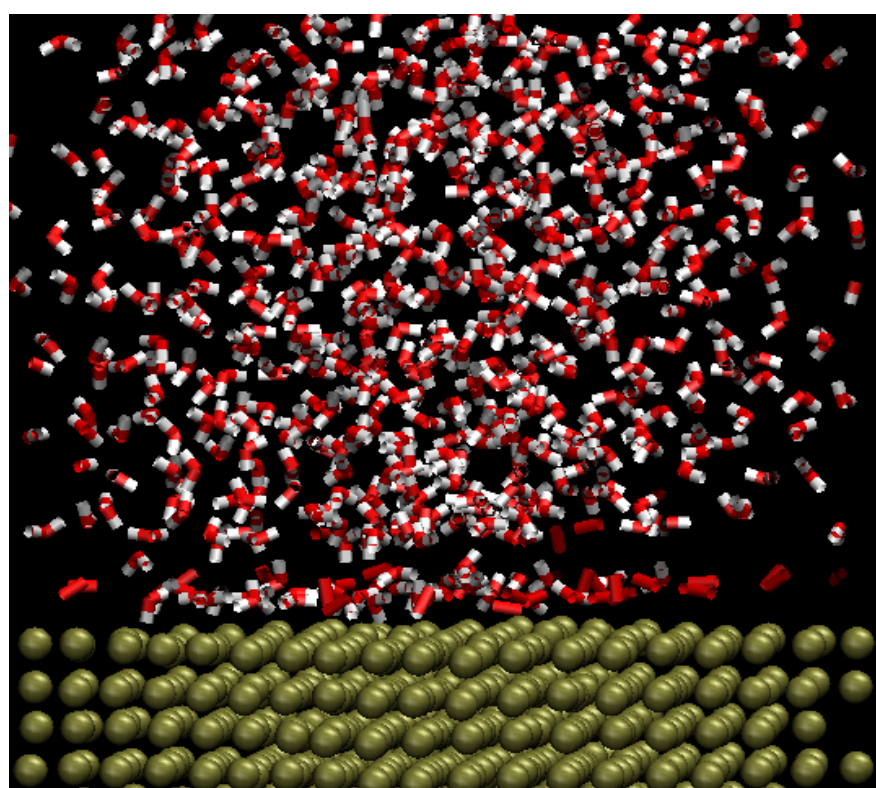
Figure S1. Snapshots of the model of Pt (111)/O₂/H₂O taken at the end of the simulation time



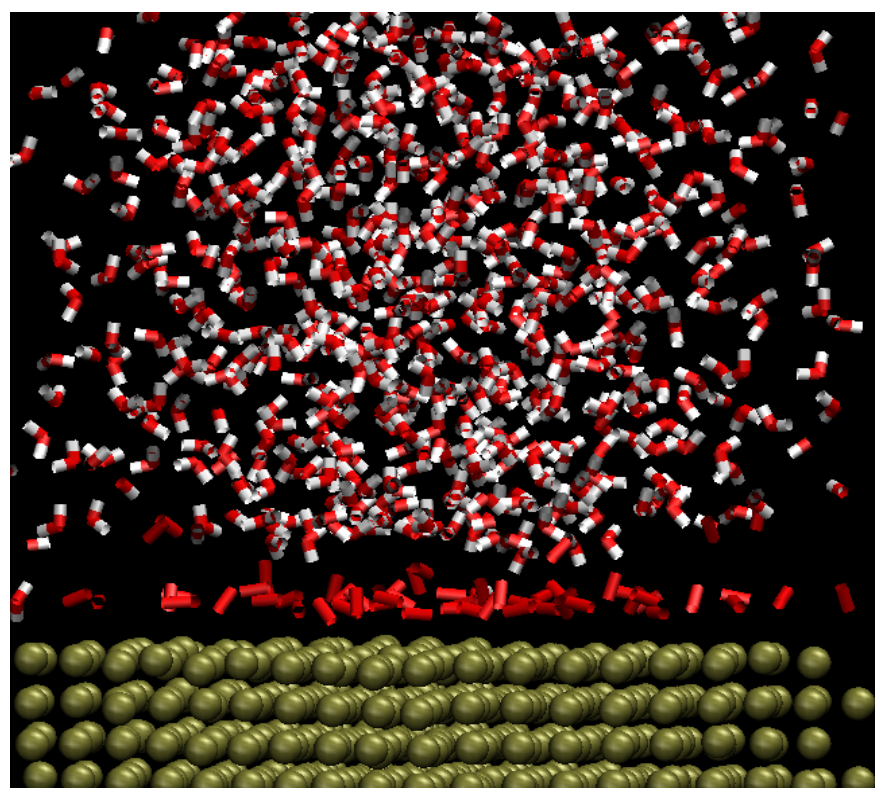
Pt (100)/16O₂/H₂O



Pt (100)/32O₂/H₂O

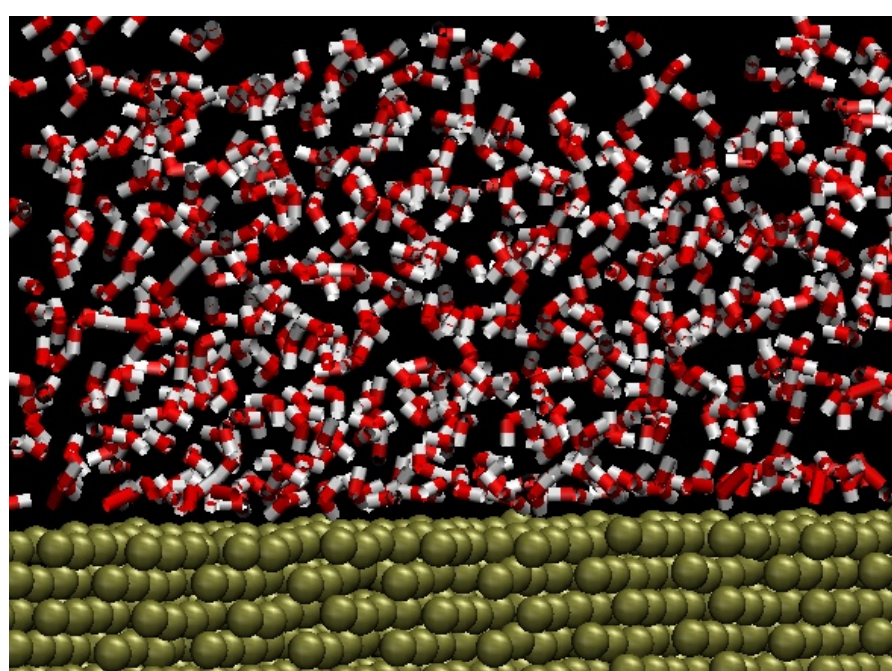


Pt (100)/48O₂/H₂O

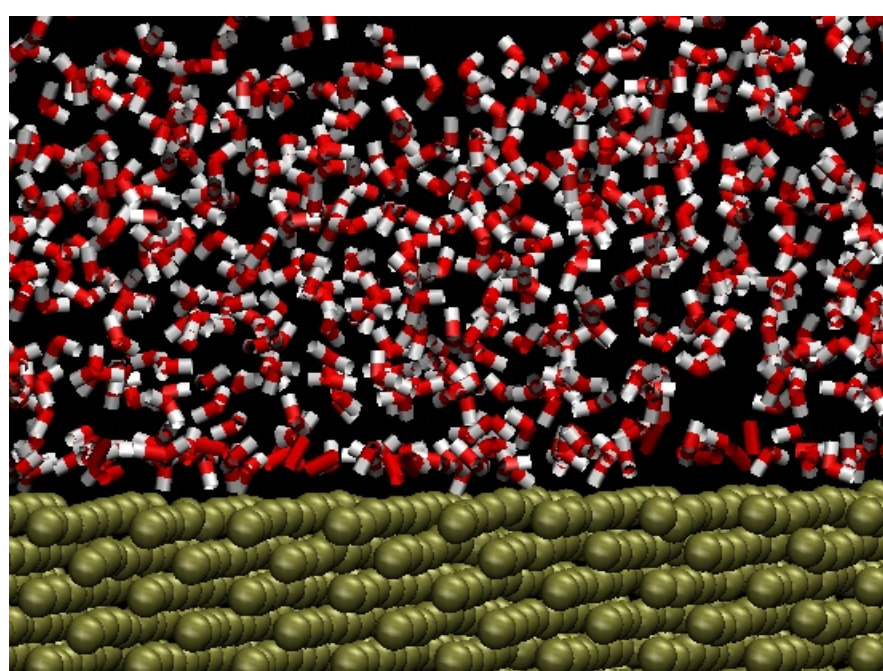


Pt (100)/64O₂/H₂O

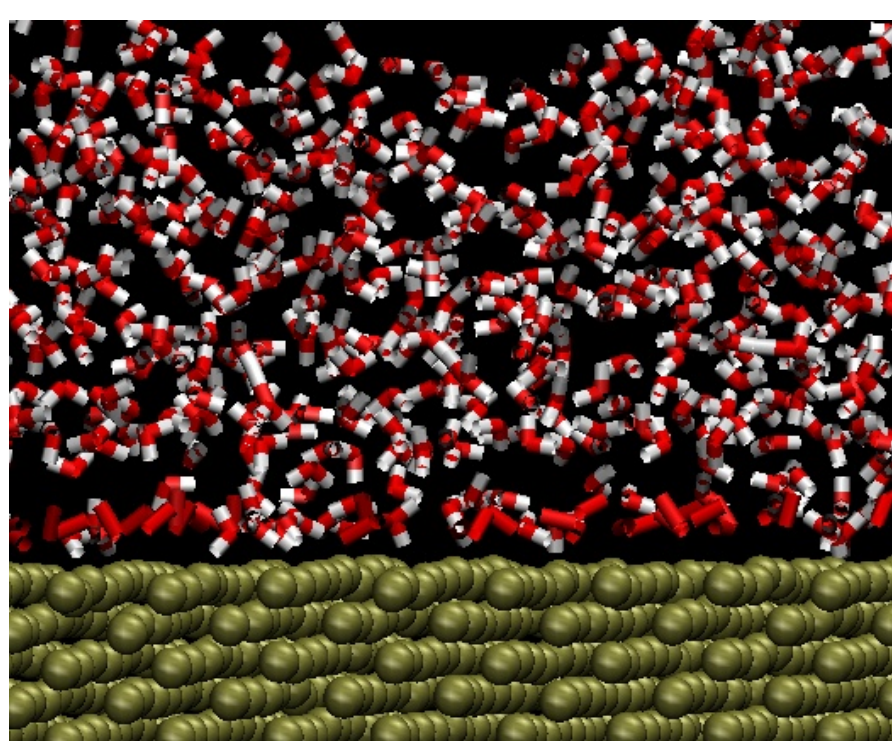
Figure S2. Snapshots of the model of Pt (100)/O₂/H₂O taken at the end of the simulation time



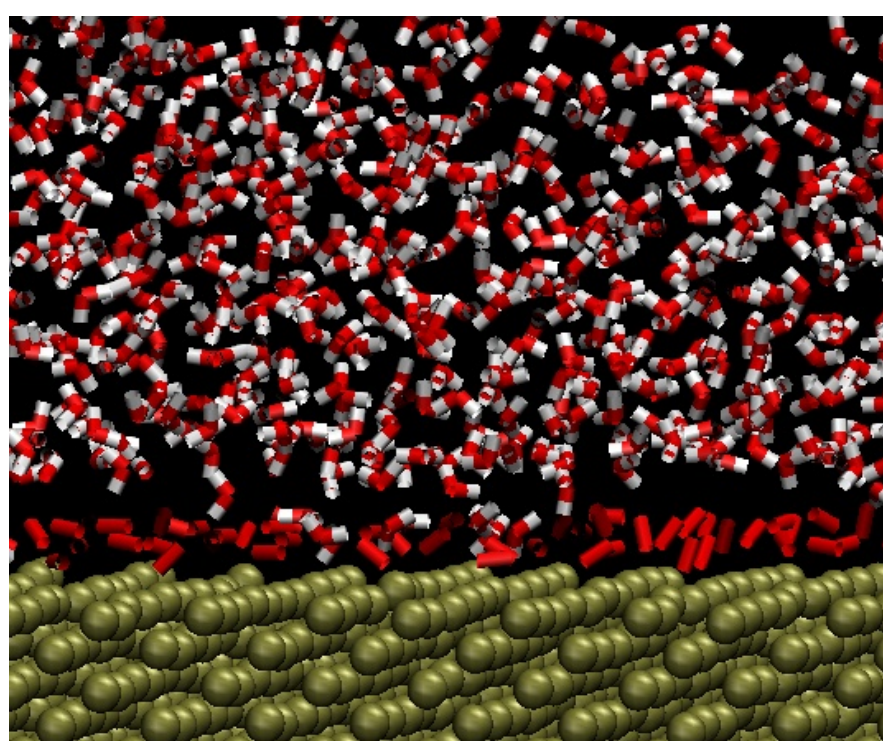
Pt (110)/16O₂/H₂O



Pt (110)/32O₂/H₂O



Pt (110)/48O₂/H₂O



Pt (110)/64O₂/H₂O

Figure S3. Snapshots of the model of Pt (110)/O₂/H₂O taken at the end of the simulation time

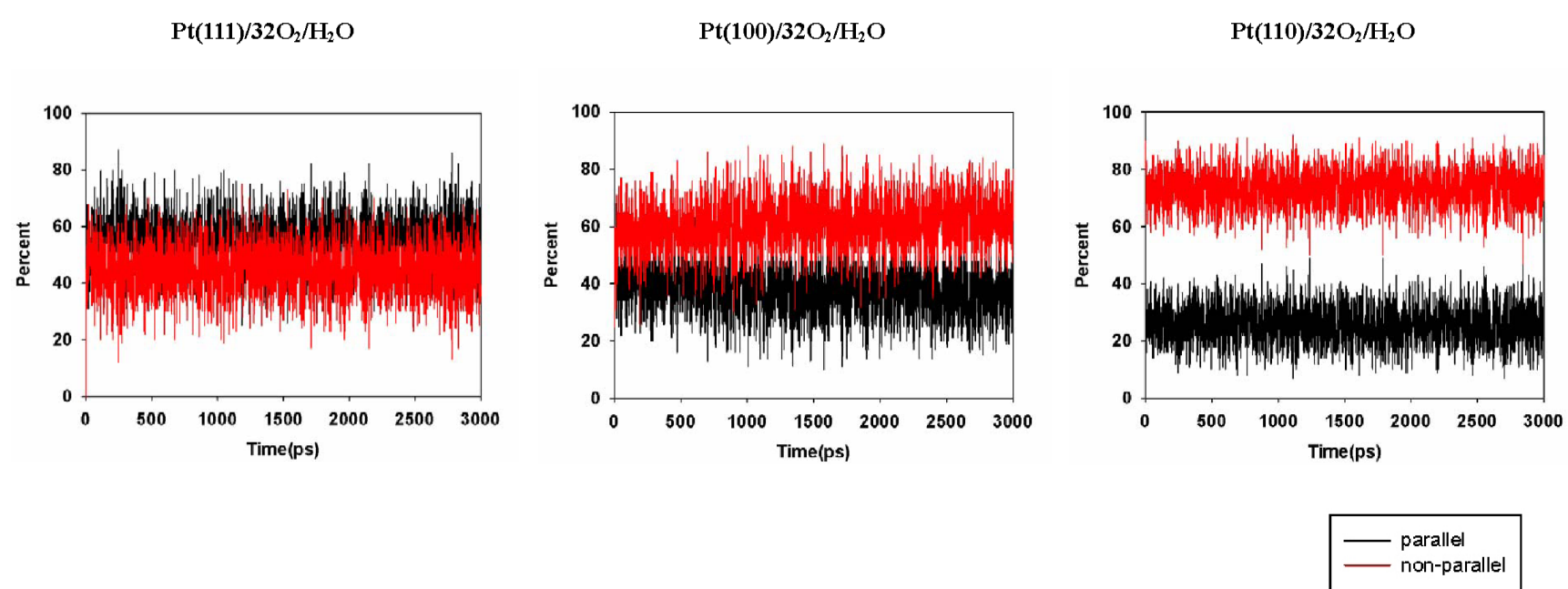


Figure S4. Distribution of the two configurations of adsorbed O₂ in models including 1200 water molecules.