Molecular dynamics simulations of surface oxidation on Pt and Pt/PtCo/Pt$_3$Co supported nanoparticles over carbon

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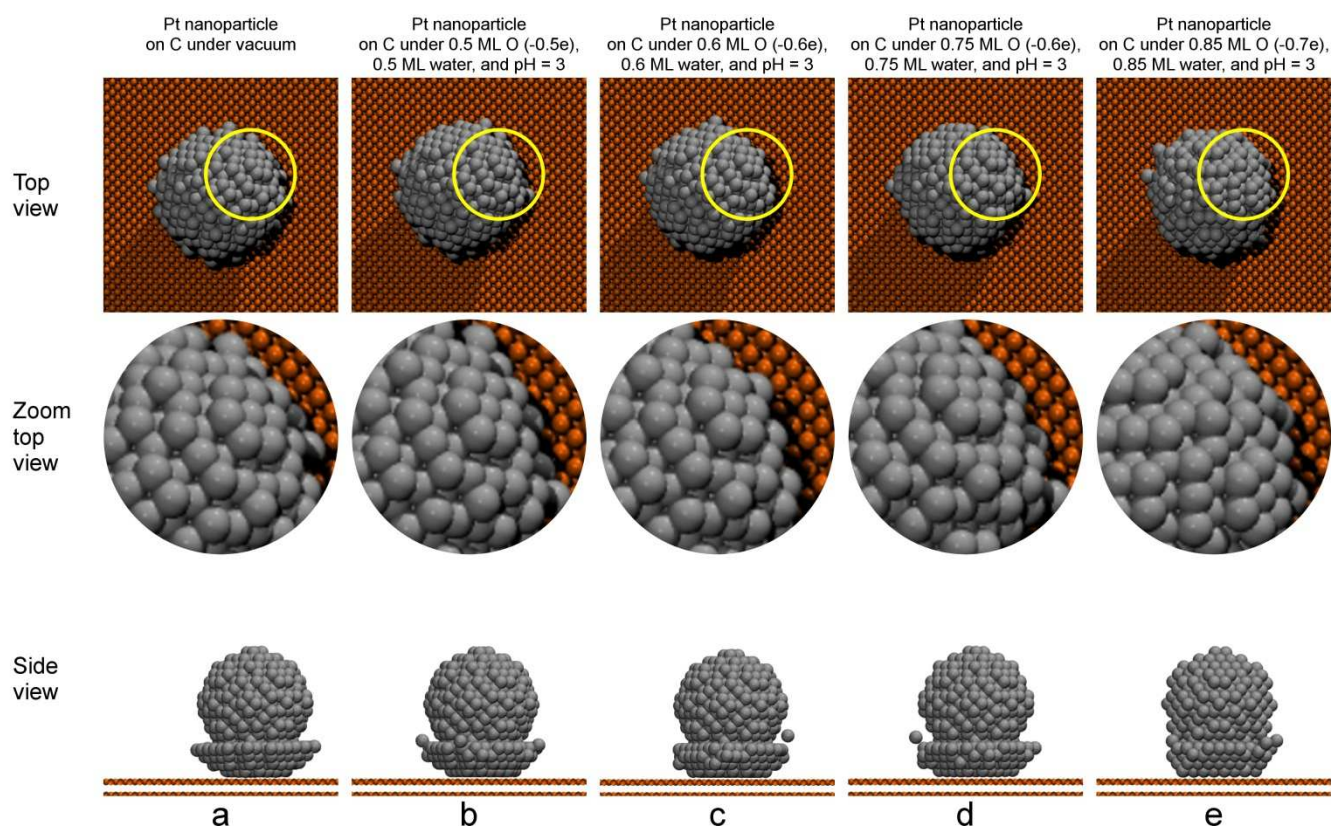*e-mail: balbuena@tamu.edu

SUPPORTING INFORMATION

Figure SI-1. Snapshots of the core and non-charged surface atoms forming the supported Pt nanoparticle on C under vacuum (a) and different coverages of oxygen and water (b-e) taken at the end of the simulation using the CF1 model and under pH =3. Color key: platinum-grey, carbon-orange.
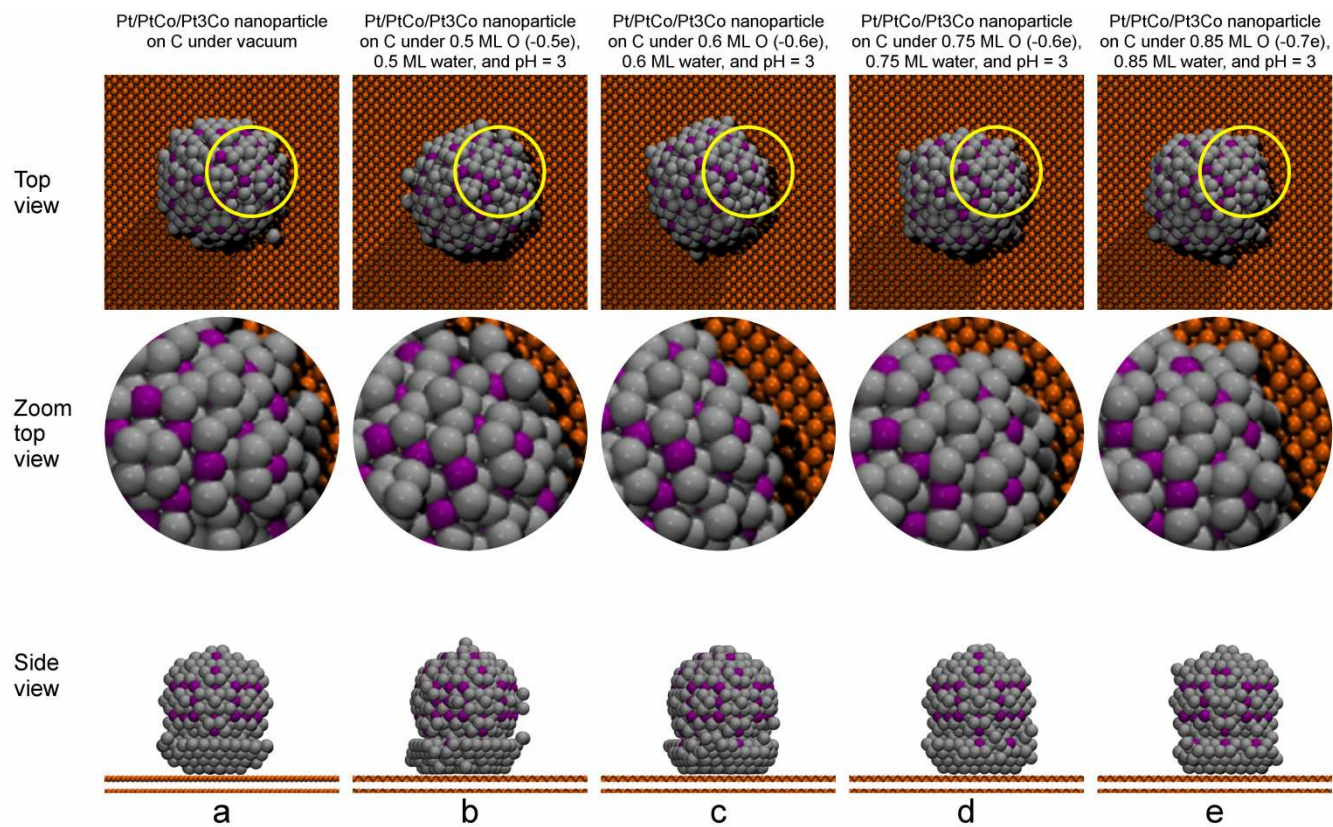
Figure SI-2. Snapshots of the core and non-charged surface atoms forming the supported Pt/PtCo/Pt3Co nanoparticle on C under vacuum (a) and different coverages of oxygen and water (b-e) taken at the end of the simulation using the CF1 model and under pH =3. Color key: platinum-grey, cobalt-purple, carbon-orange.
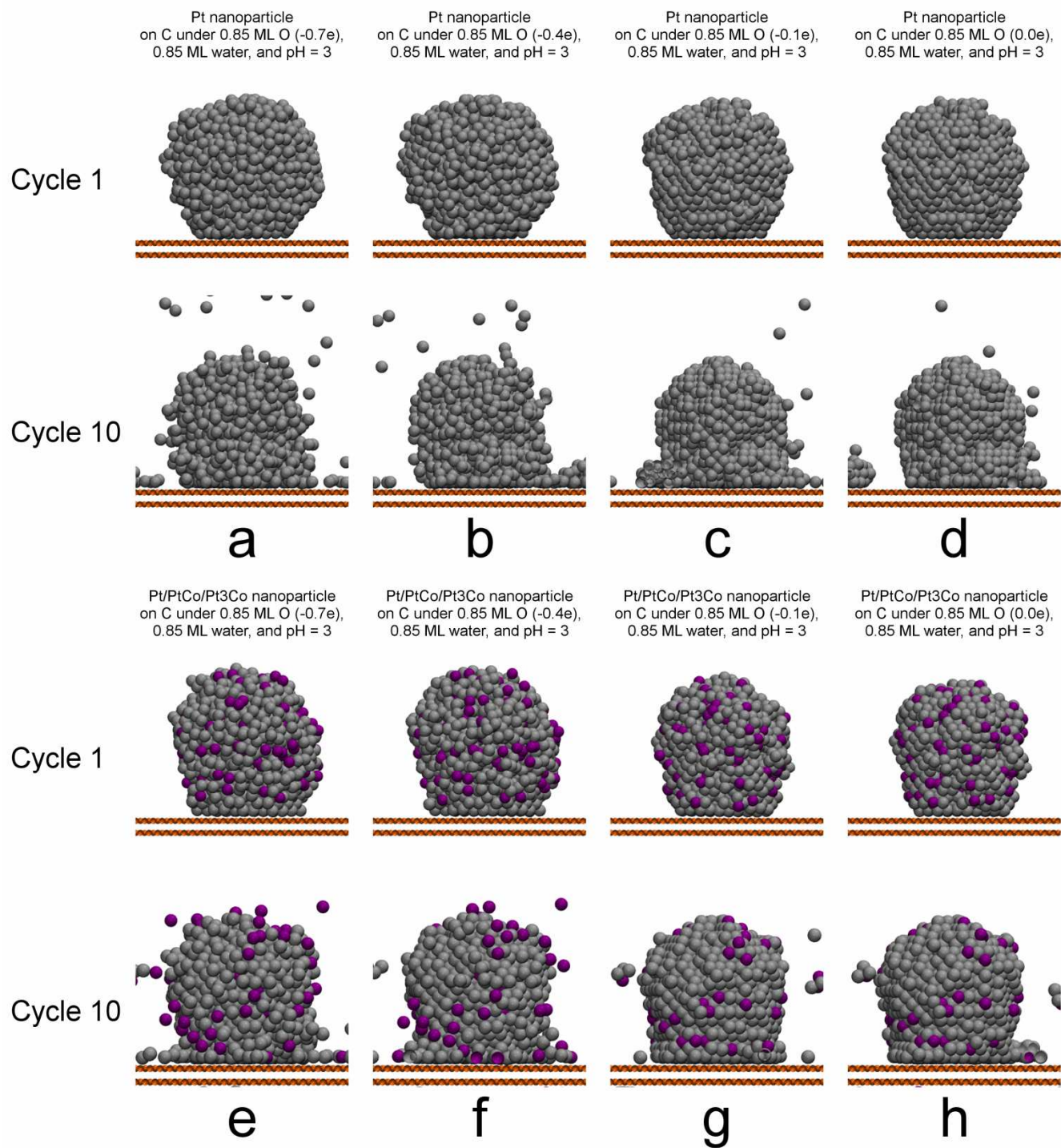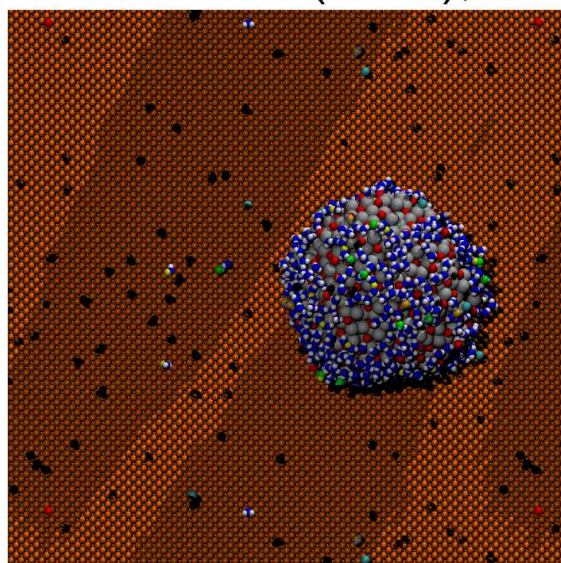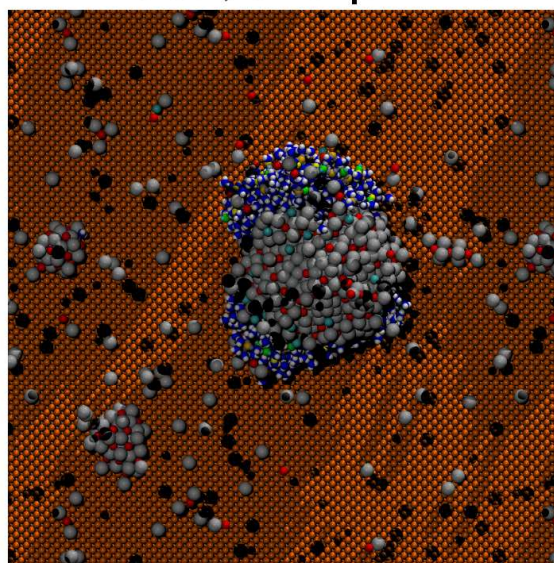
Figure SI-3. Snapshots of the supported Pt(a-d) and Pt/PtCo/Pt3Co(e-h) nanoparticles on C under 0.85 ML of oxygen and water, and pH = 3 taken at the end of the simulation after 1 and 10 reduction-oxidation cycles. All the adsorbates are hidden. Color key: platinum-grey, cobalt-purple, carbon-orange.

Pt nanoparticle on C under
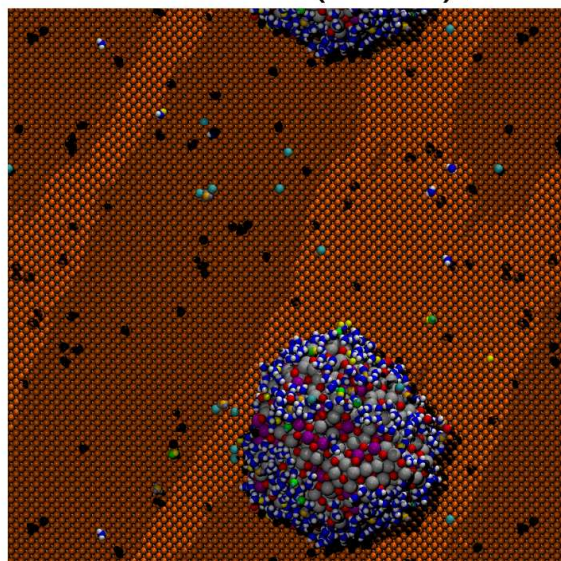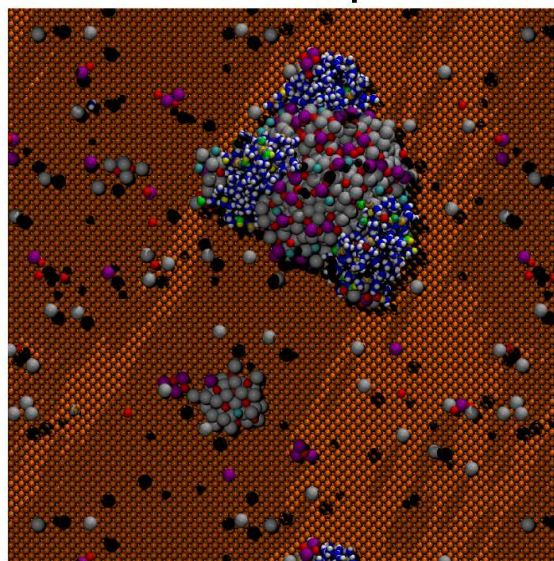## 0.85 ML O (-0.7e), 0.85 ML water, and pH = 3

cycle 1

cycle 10

Pt/PtCo/Pt3Co nanoparticle on C under
0.85 ML O (-0.7e), 0.85 ML water, and pH = 3

cycle 1

cycle 10

Figure SI-4. Snapshots of the supported Pt (top row) and Pt/PtCo/Pt3Co (bottom row) nanoparticles on C under 0.85 ML of oxygen and water, and pH = 3 taken at the end of the simulation after 1 and 10 reduction-oxidation cycles. Color key: platinum-grey, cobalt-purple, oxygen-red, cation-yellow, OH-green, H_2O-blue and white, H_3O-orange and purple, anion-cyan, carbon-orange.
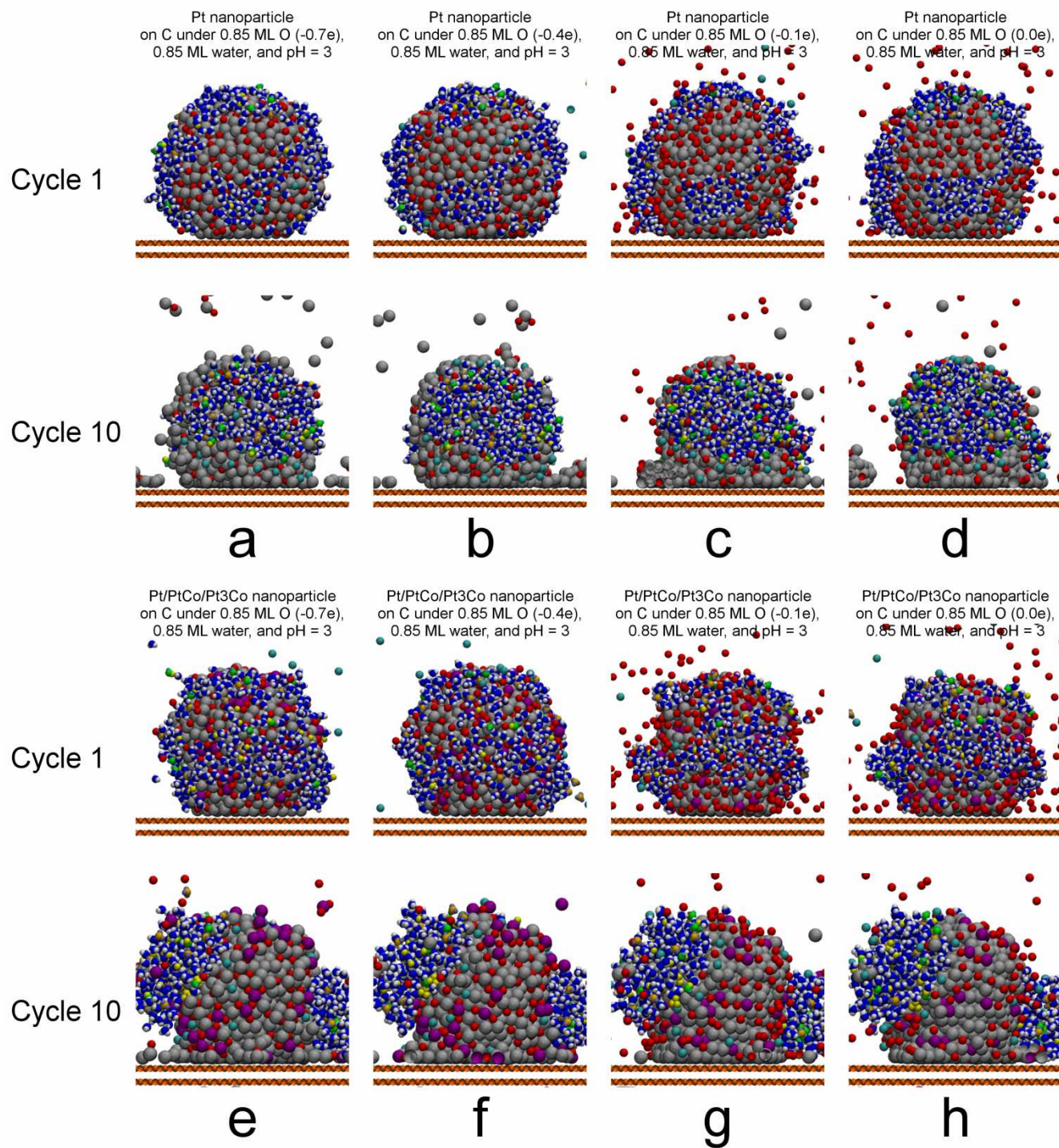
Figure SI-5. Snapshots of the supported Pt(a-d) and Pt/PtCo/Pt3Co(e-h) nanoparticles on C under 0.85 ML of oxygen and water, and pH = 3 taken at the end of the simulation after 1 and 10 reduction-oxidation cycles. Color key: platinum-grey, cobalt-purple, oxygen-red, cation-yellow, OH-green, H$_2$O-blue and white, H$_3$O-orange and purple, anion-cyan, carbon-orange.
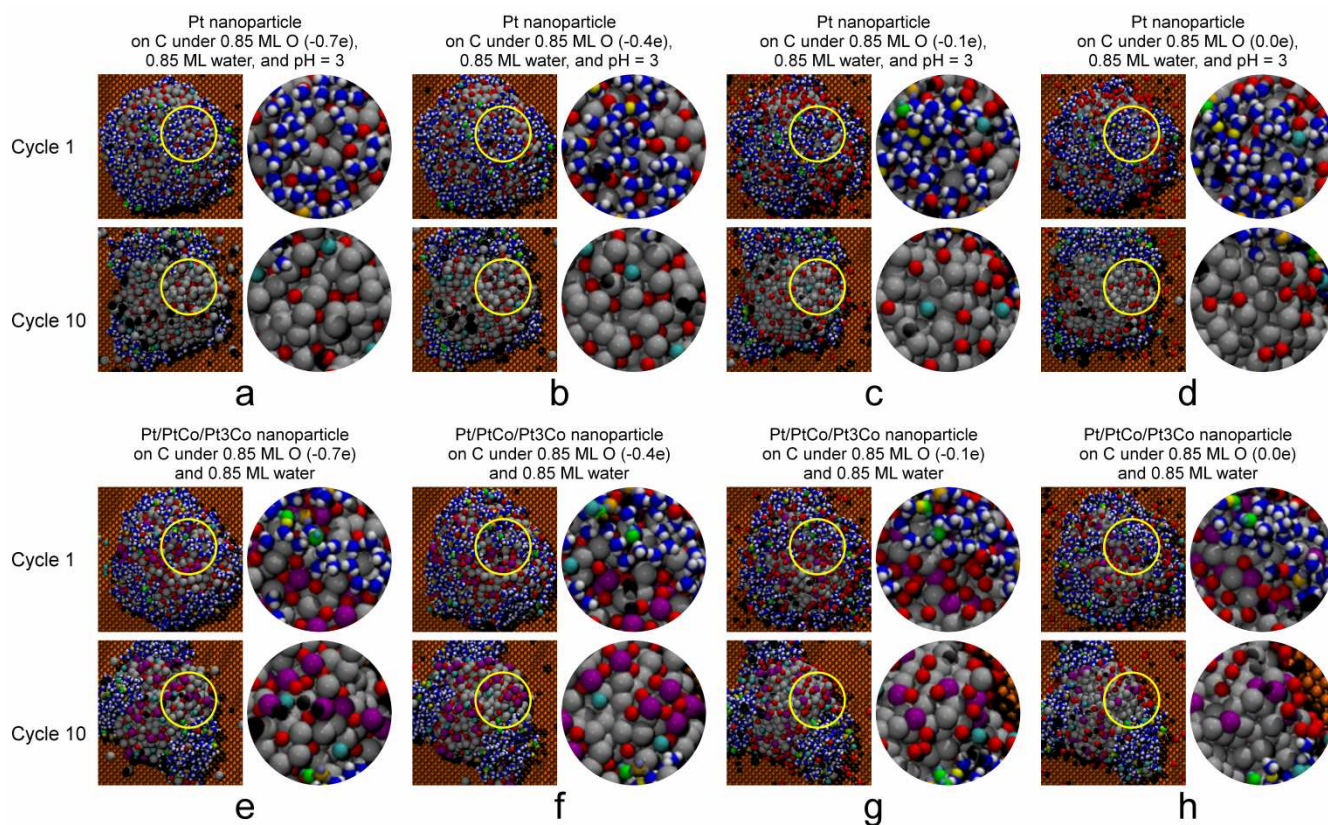
Figure SI-6. Snapshots of the supported Pt(a-d) and Pt/PtCo/Pt3Co(e-h) nanoparticles on C under 0.85 ML of oxygen and water, and pH = 3 taken at the end of the simulation after 1 and 10 reduction-oxidation cycles. Color key: platinum-grey, cobalt-purple, oxygen-red, cation-yellow, OH-green, H_2O-blue and white, H_3O-orange and purple, anion-cyan, carbon-orange.