Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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Oxygen Adsorption on High-Index Faceted Pt Nanoparticles

(Supplementary Information)

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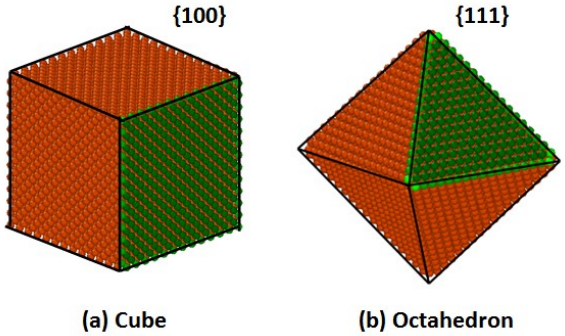

Figure S1. Schematic illustration of two low-index faceted Pt nanoparticles: (a) cube and (b) octahedron, respectively enclosed by {100} and {111} facets. The numbers of atoms in (a) and (b) are respectively 8788 and 4572. The facet boundaries are highlighted by the black solid lines. Varying shades of green colors are adopted to denote atoms with different CNs: the lighter green corresponds to the lower CN.

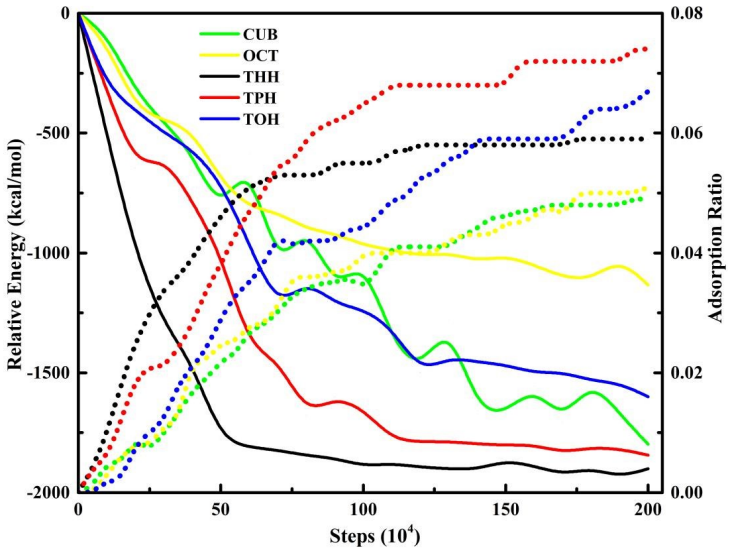

Figure S2. Equilibration of the test simulations performed at T = 300 K. Two low-index faceted nanoparticles (cube and octahedron) and three high-index faceted nanoparticles (THH, TPH, and TOH) with the similar diameter (~ 5 nm) are set to be surrounded by 50 oxygen molecules. The solid lines correspond to the relative energies, and the dashed lines denote the corresponding adsorption ratios.

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