DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle

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Minimised Geometries

Fig. S1: IS, TS and FS structures for O$_2$ dissociation on Pt$_{116}$, when O$_2$ is located at position 8. Only the top two layers of metal atoms are shown.

Fig. S2: IS, TS and FS structures for O$_2$ dissociation on Pt$_{116}$, when O$_2$ is located at position 9. Only the top two layers of metal atoms are shown.
Fig. S3: IS, TS and FS structures for O\textsubscript{2} dissociation on Pt\textsubscript{116}, when O\textsubscript{2} is located at position 10. Only the top two layers of metal atoms are shown.

Fig. S4: IS, TS and FS structures for O\textsubscript{2} dissociation on Pt\textsubscript{116}, when O\textsubscript{2} is located at position 11. Only the top two layers of metal atoms are shown.
Fig. S5: IS, TS and FS structures for O\textsubscript{2} dissociation on Pt\textsubscript{116}, when O\textsubscript{2} is located at position 12. Only the top two layers of metal atoms are shown.

Fig. S6: IS, TS and FS structures for O\textsubscript{2} dissociation on Pt\textsubscript{116}, when O\textsubscript{2} is located at position 14. Only the top two layers of metal atoms are shown.
Fig. S7: IS, TS and FS structures for O\textsubscript{2} dissociation on the extended Pt(111) surface.
**Charge Density Difference**

The charge density difference plots are shown in Fig. S8–S14. These are generated by subtracting from the charge (electron) density of the total system Pt$_{116}$–O$_2$, the charge densities of its fragments: Pt$_{116}$ and O$_2$ (or O + O). The charge densities of the Pt$_{116}$ and O$_2$ fragments are calculated with the positions of atoms optimized for the total system. The pink surface indicates the depletion of electron density, while the green surface indicates the accumulation of electron density.

Fig. S8: IS, TS and FS charge density difference plots for O$_2$ on site 8 of the Pt$_{116}$ particle.

Fig. S9: IS, TS and FS charge density difference plots for O$_2$ on site 9 of the Pt$_{116}$ particle.

Fig. S10: IS, TS and FS charge density difference plots for O$_2$ on site 10 of the Pt$_{116}$ particle.
Fig. S11: IS, TS and FS charge density difference plots for $O_2$ on site 11 of the Pt$_{116}$ particle.

Fig. S12: IS, TS and FS charge density difference plots for $O_2$ on site 12 of the Pt$_{116}$ particle.

Fig. S13: IS, TS and FS charge density difference plots for $O_2$ on site 14 of the Pt$_{116}$ particle.
Fig. S14: IS, TS and FS charge density difference plots for the extended Pt(111) surface.