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_2 dissociation on Pt_{116} , when O_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_2 dissociation on Pt_{116} , when O_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_2 dissociation on Pt_{116} , when O_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_2 dissociation on Pt_{116} , when O_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_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.