A DFT study of oxygen dissociation on platinum based nanoparticles

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Supplementary Information

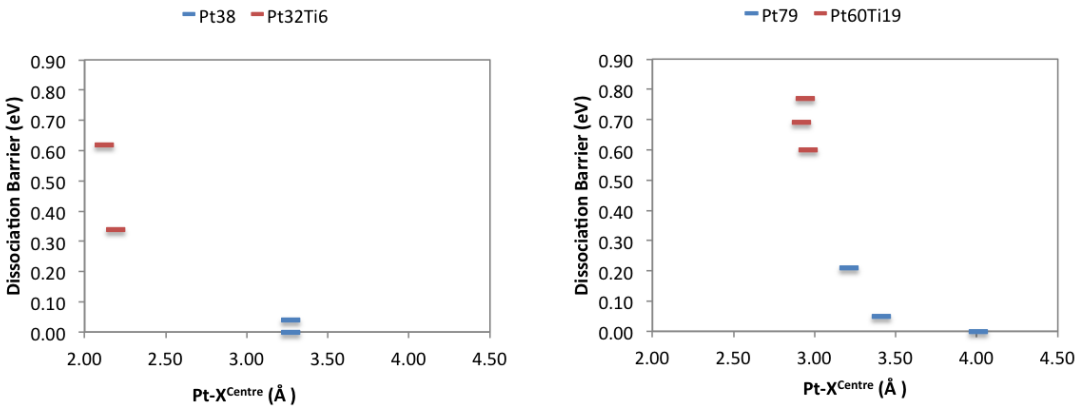

Fig. S1 Plot of Pt-X^{centre} against dissociation barrier at the IS for 38 atom (left) and 79 atom (right) clusters.

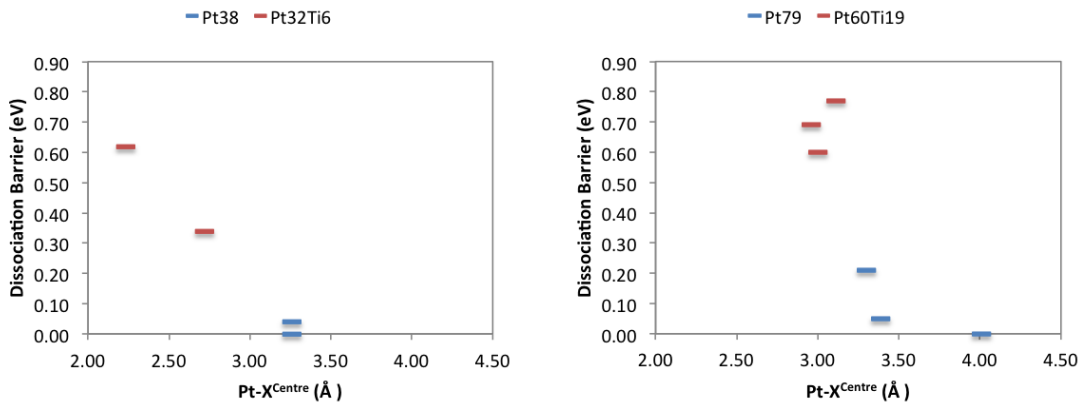

Fig. S2 Plot of Pt-X^{centre} against dissociation barrier at the TS for 38 atom (left) and 79 atom (right) clusters.

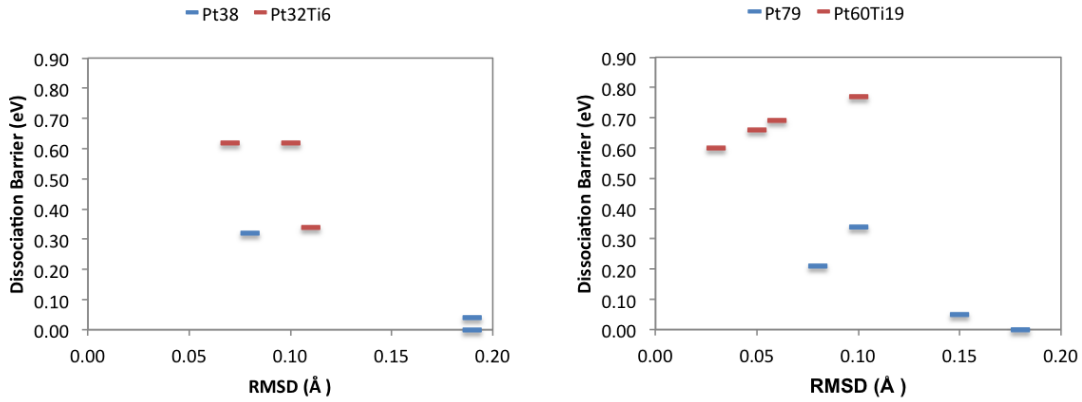

Fig. S3 Plot of RMSD against dissociation barrier at the TS for 38 atom (left) and 79 atom (right) clusters.

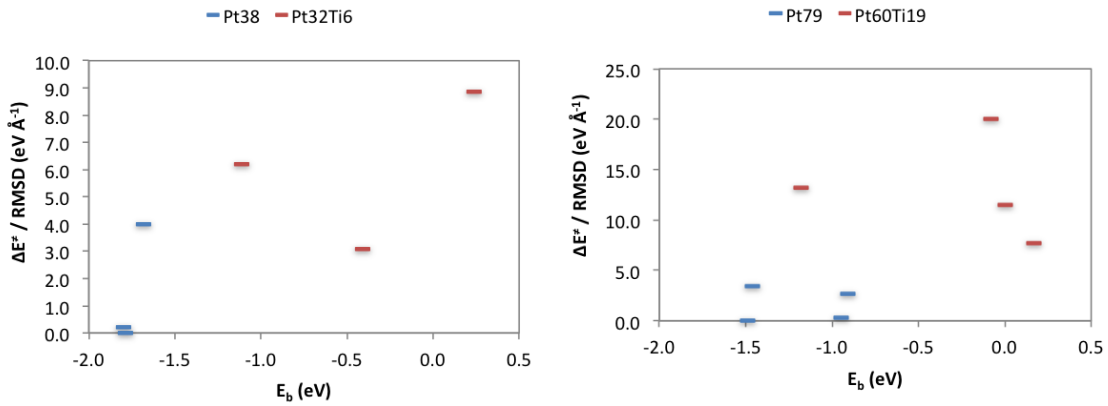

Fig. S4 Plot of $\Delta E^{\neq}/RMSD$ against E_b at the TS for 38 atom (left) and 79 atom (right) clusters.

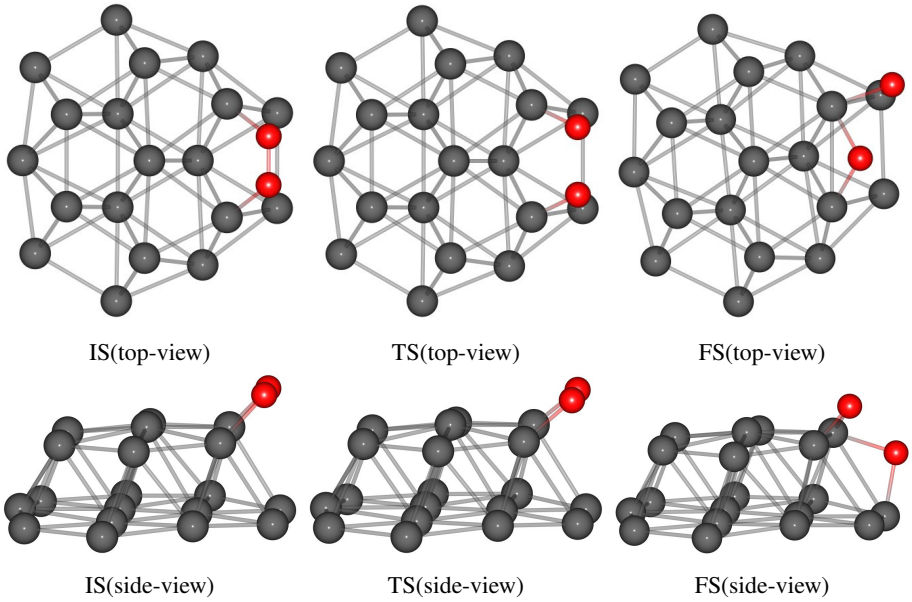

Fig. S5 IS, TS and FS structures for O_2 dissociation on Pt_{38}, when O_2 is located at **position 5**. Only top two layers of metal atoms are shown.

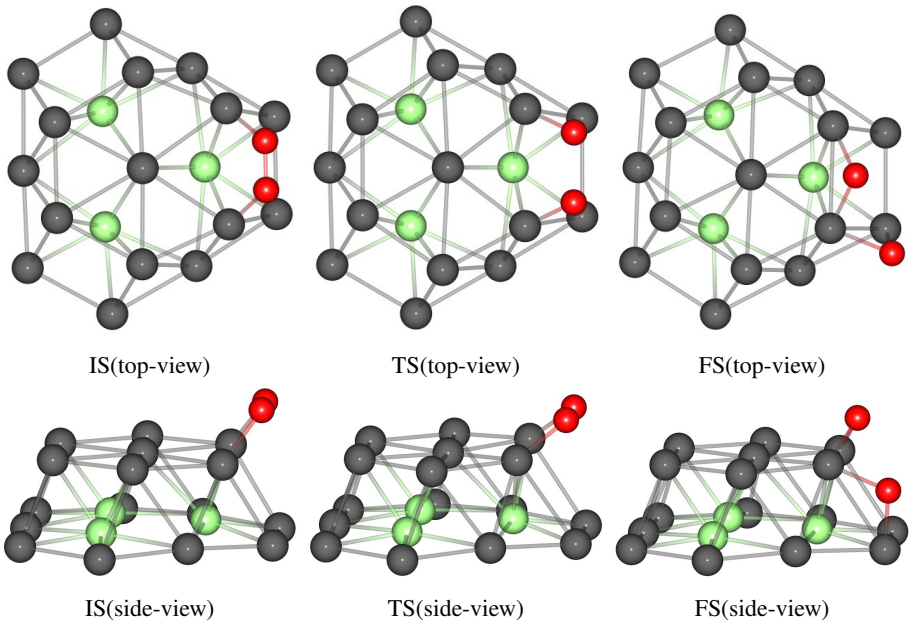

Fig. S6 IS, TS and FS structures for O_2 dissociation on $Pt_{32}Ti_6$, when O_2 is located at **position 5**. Only top two layers of metal atoms are shown.

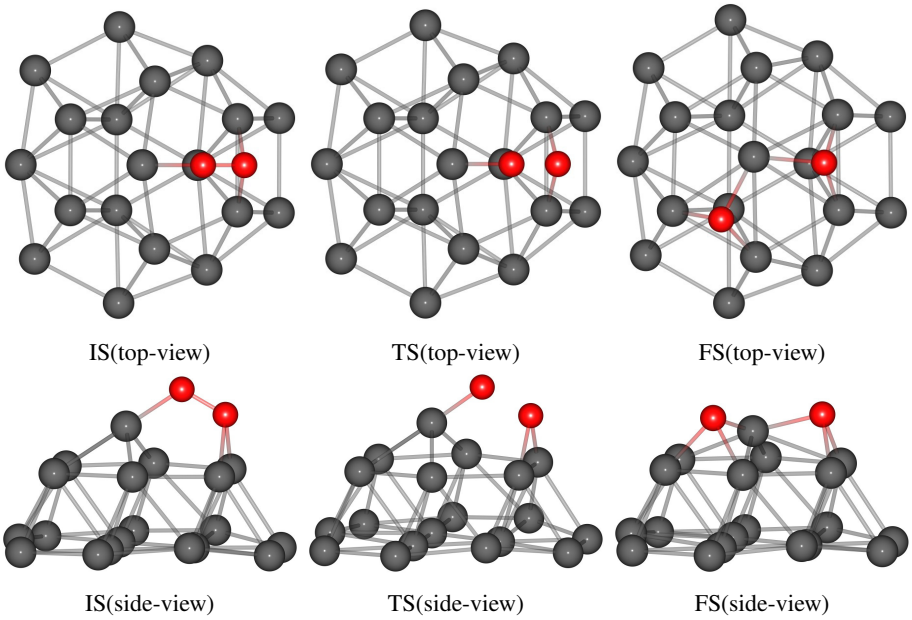

Fig. S7 IS, TS and FS structures for O_2 dissociation on Pt_{38}, when O_2 is located at **position 6**. Only top two layers of metal atoms are shown.

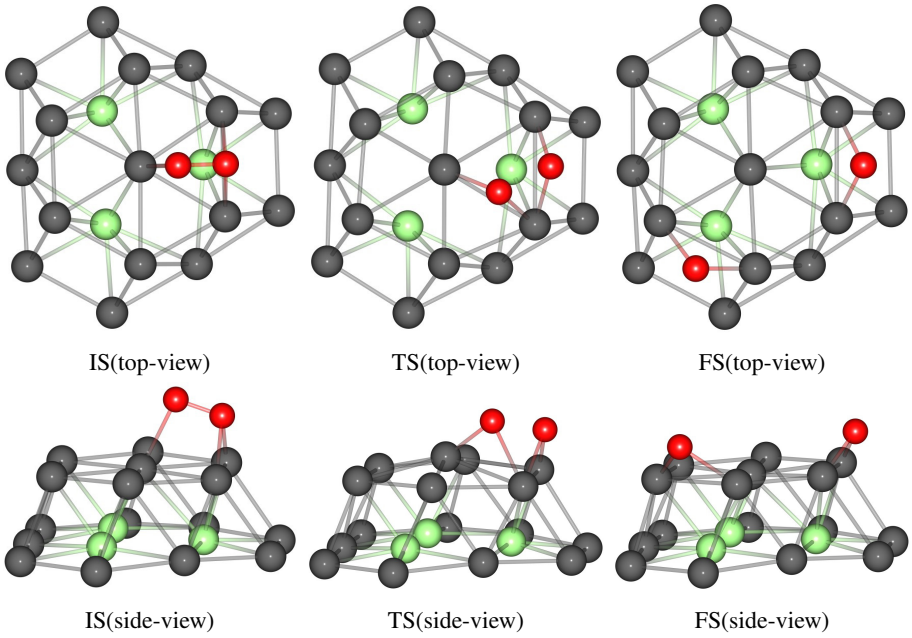

Fig. S8 IS, TS and FS structures for O_2 dissociation on $Pt_{32}Ti_6$, when O_2 is located at **position 6**. Only top two layers of metal atoms are shown.

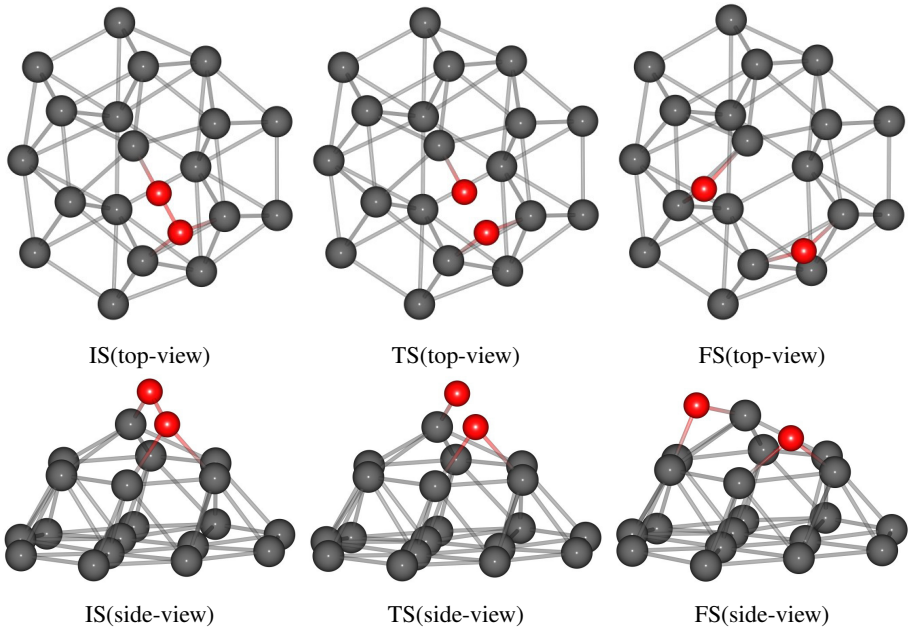

Fig. S9 IS, TS and FS structures for O_2 dissociation on Pt_{38}, when O_2 is located at **position 7**. Only top two layers of metal atoms are shown.

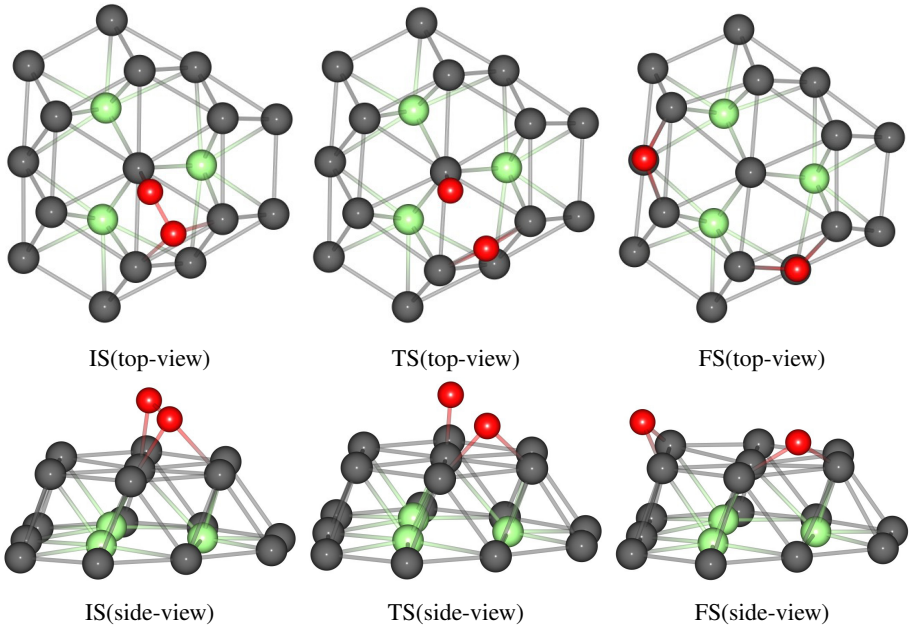

Fig. S10 IS, TS and FS structures for O_2 dissociation on $Pt_{32}Ti_6$, when O_2 is located at **position 7**. Only top two layers of metal atoms are shown.

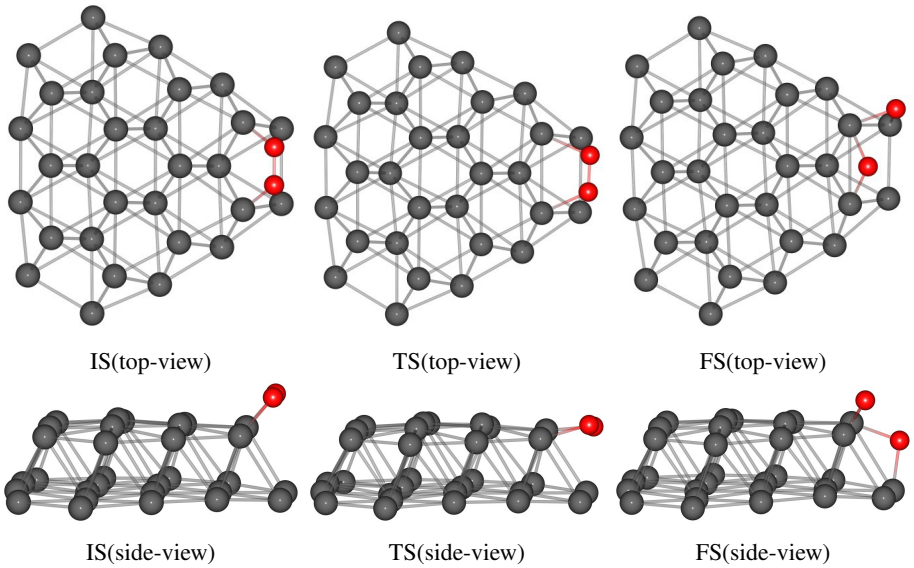

Fig. S11 IS, TS and FS structures for O_2 dissociation on Pt_{79}, when O_2 is located at **position 8**. Only top two layers of metal atoms are shown.

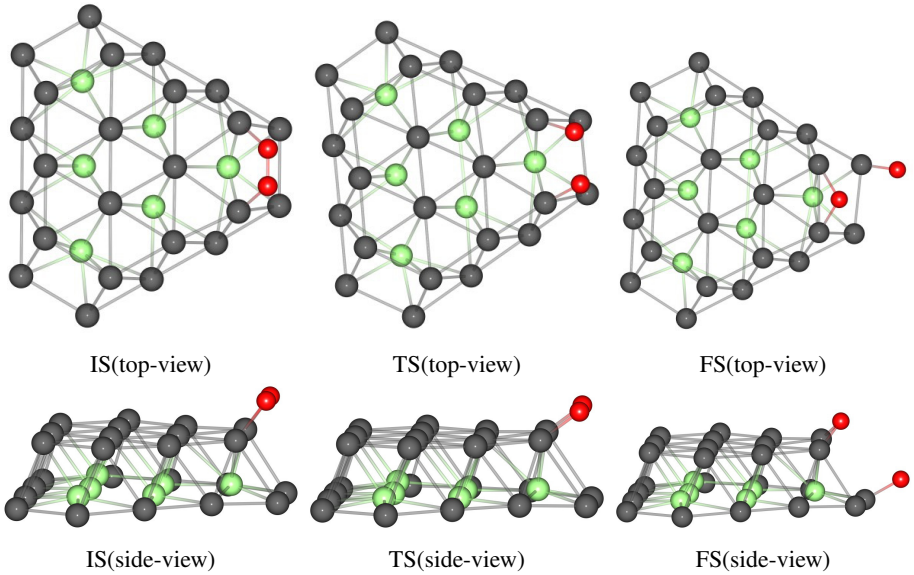

Fig. S12 IS, TS and FS structures for O_2 dissociation on $Pt_{60}Ti_{19}$, when O_2 is located at **position 8**. Only top two layers of metal atoms are shown.

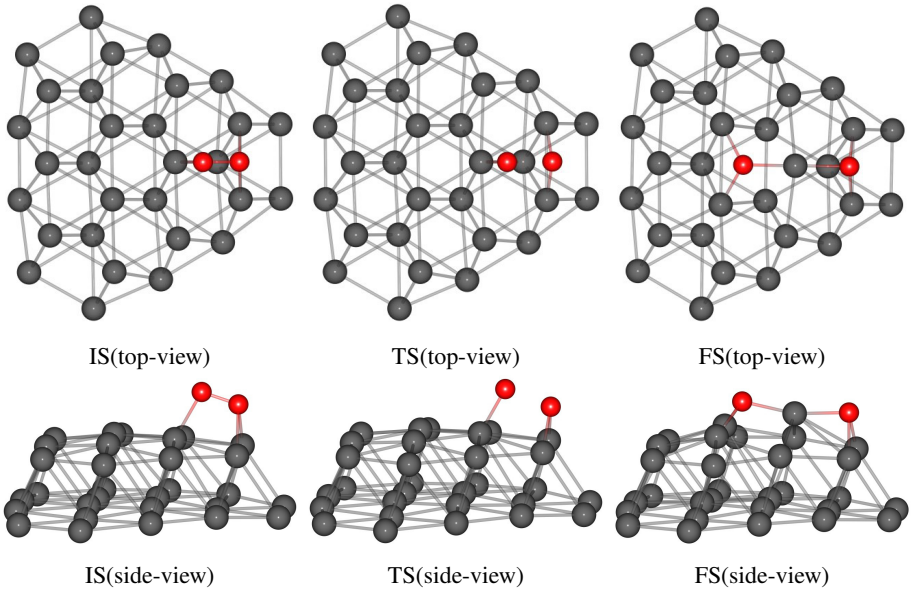

Fig. S13 IS, TS and FS structures for O_2 dissociation on Pt_{79}, when O_2 is located at **position 9**. Only top two layers of metal atoms are shown.

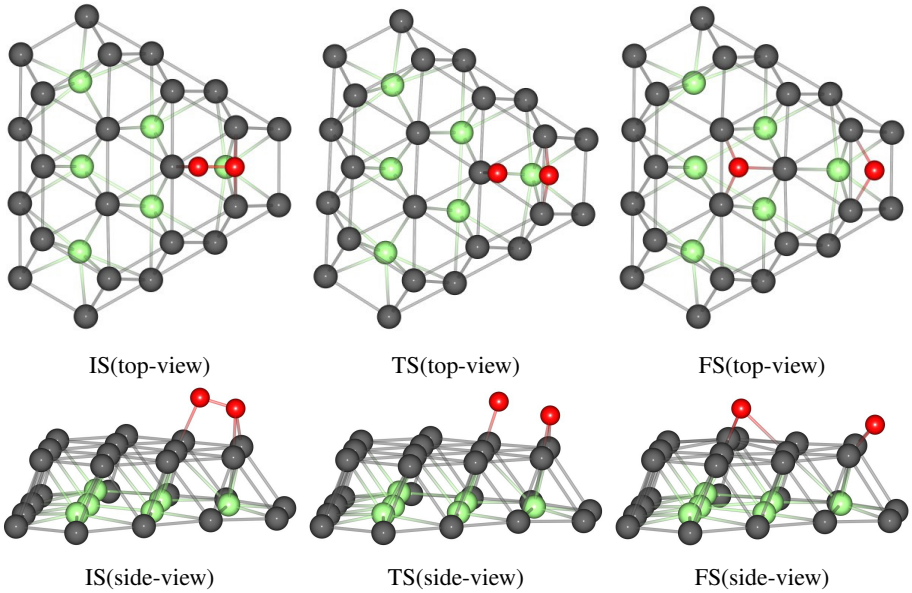

Fig. S14 IS, TS and FS structures for O_2 dissociation on $Pt_{60}Ti_{19}$, when O_2 is located at **position 9**. Only top two layers of metal atoms are shown.

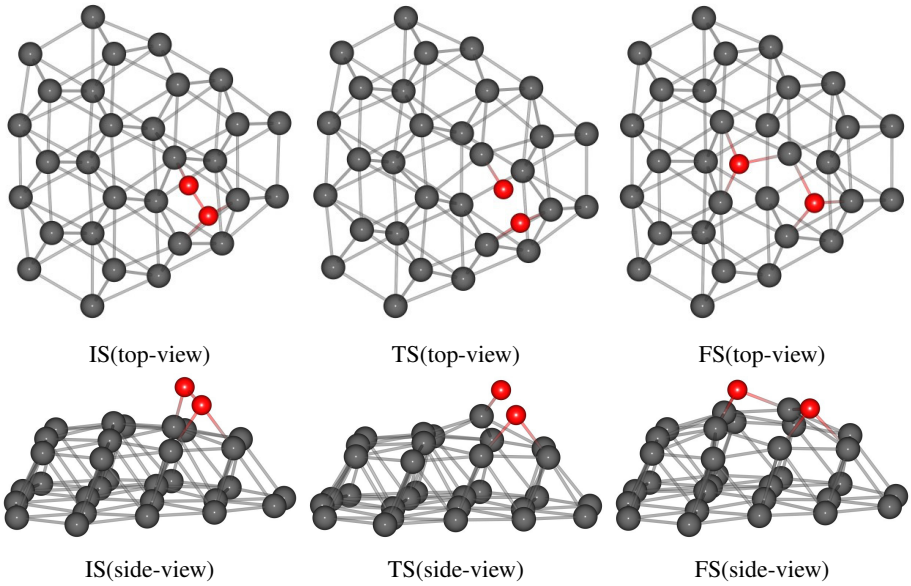

Fig. S15 IS, TS and FS structures for O_2 dissociation on Pt_{79}, when O_2 is located at **position 10**. Only top two layers of metal atoms are shown.

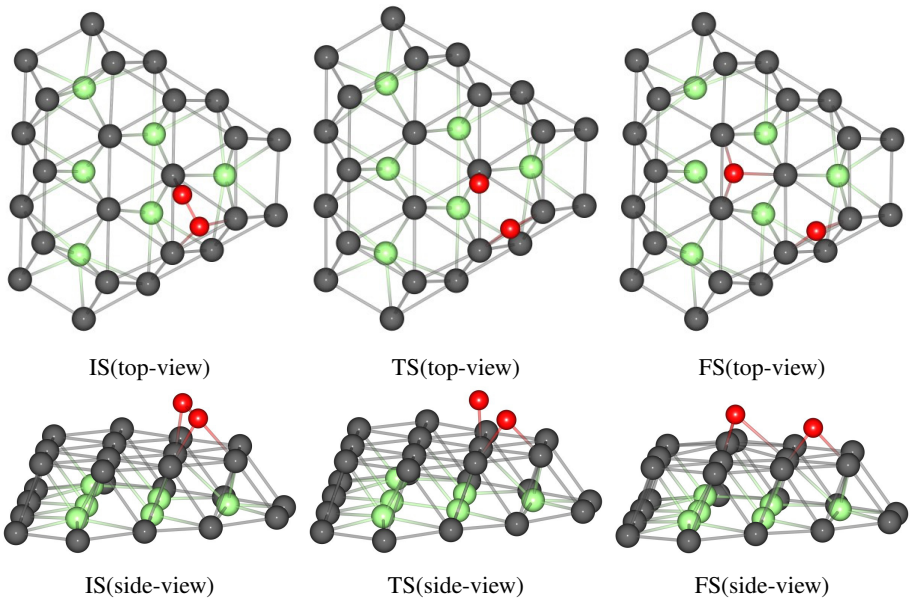

Fig. S16 IS, TS and FS structures for O_2 dissociation on $Pt_{60}Ti_{19}$, when O_2 is located at **position 10**. Only top two layers of metal atoms are shown.

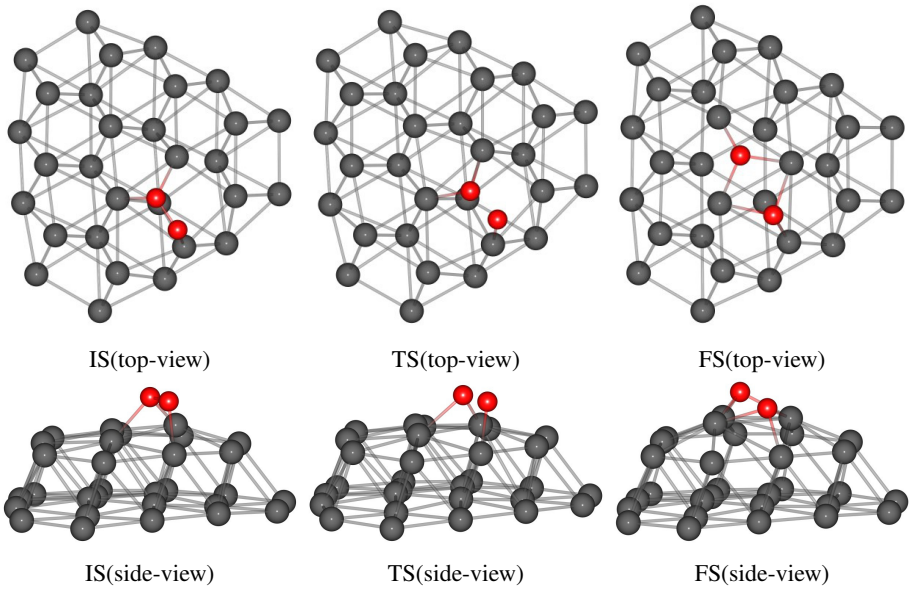

Fig. S17 IS, TS and FS structures for O_2 dissociation on Pt_{79}, when O_2 is located at **position 11**. Only top two layers of metal atoms are shown.

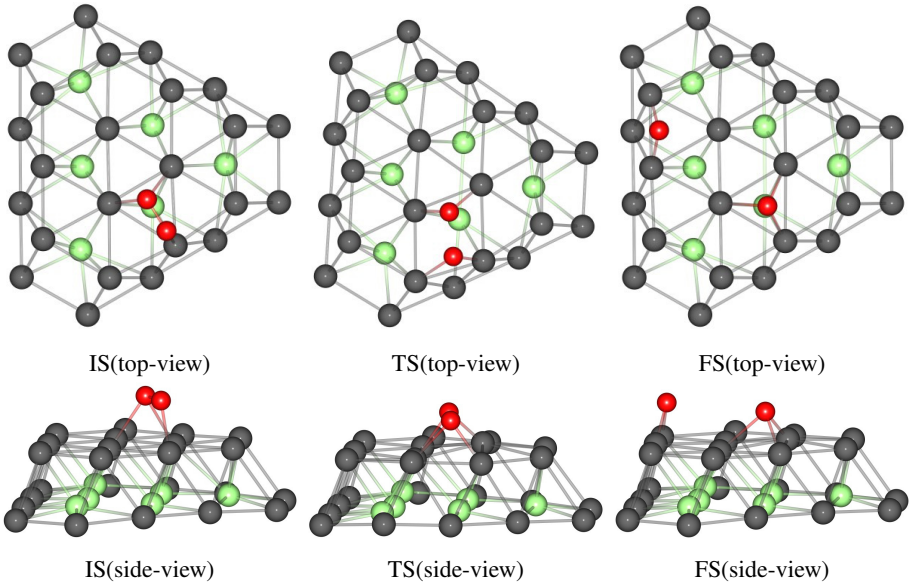

Fig. S18 IS, TS and FS structures for O_2 dissociation on $Pt_{60}Ti_{19}$, when O_2 is located at **position 11**. Only top two layers of metal atoms are shown.