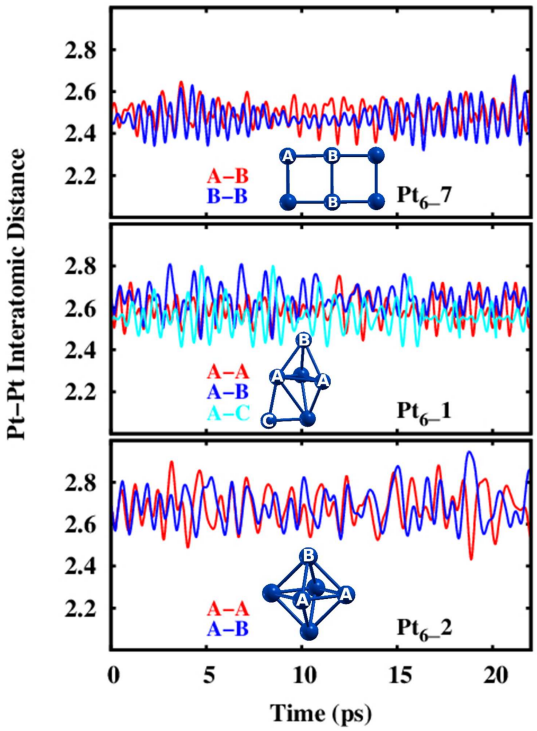
Supporting Information For:

# Tailoring the electronic properties of platinum and gold-platinum nanocatalysts towards enhanced $O_2$ activation.

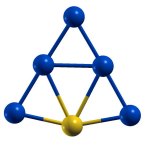
Krati Joshi and Sailaja Krishnamurty
*Functional Materials Division, CSIR-Central Electrochemical Research Institute, Karaikudi-630 006, India*



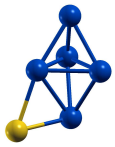

Supp-Fig. 1

Inter-atomic bond Length fluctuations ($\AA$) in various $Pt_6$ conformations as a function of time (ps) at 350 K.

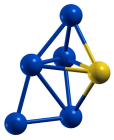
**$Au_1Pt_5$**



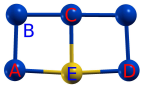
**$Au_1Pt_5$-GS_2**



**$Au_1Pt_5$-1_2**

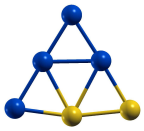


**$Au_1Pt_5$-1_3**

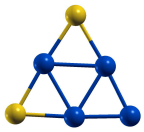



**$Au_1Pt_5$-7_2**

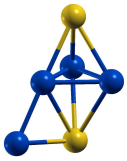
**$Au_2Pt_4$**



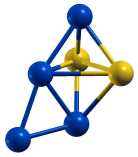
**$Au_2Pt_4$-GS_1**



**$Au_2Pt_4$-GS_2**



**$Au_2Pt_4$-1_1**



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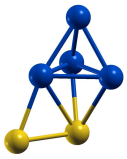
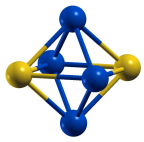
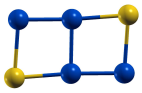


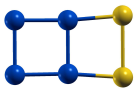
**$Au_2Pt_4$-1_4**



**$Au_2Pt_4$-2_1**

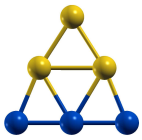


**$Au_2Pt_4$-7_1**

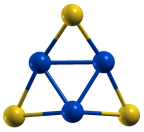


**$Au_2Pt_4$-7_3**

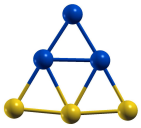
**$Au_3Pt_3$**



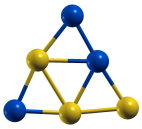
**$Au_3Pt_3$-GS_2**



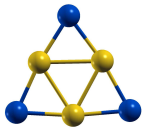
**$Au_3Pt_3$-GS_3**



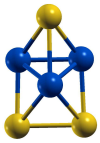
**$Au_3Pt_3$-GS_4**



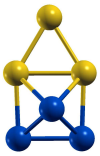
**$Au_3Pt_3$-GS_5**



**$Au_3Pt_3$-GS_6**

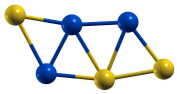


**$Au_3Pt_3$-1_1**

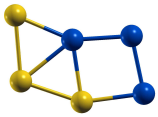


**$Au_3Pt_3$-1_2**

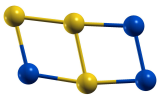
**$Au_3Pt_3$-1_4**



**$Au_3Pt_3$-7_1**

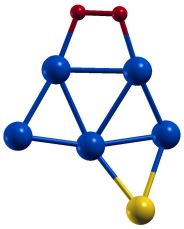


**$Au_3Pt_3$-7_3**



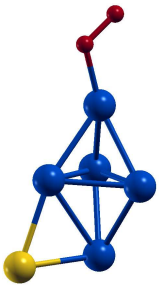
**$Au_3Pt_3$-7_4**

Supp-Fig. 2
Putative models of six atom $Au_nPt_m$ (n,m = 1,5; 2,4; 3,3) clusters.



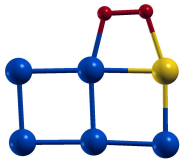
**$Au_1Pt_5$-GS_1-D**

**(1.37 Å)**



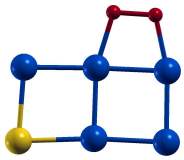
**$Au_1Pt_5$-1_2-A**

**(1.28 Å)**



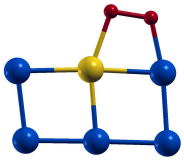
**$Au_1Pt_5$-7_1-D**

**(1.43 Å)**



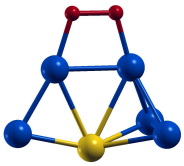
**$Au_1Pt_5$-7_1-E**

**(1.46 Å)**



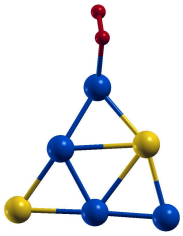
**$Au_1Pt_5$-7_2-E**

**(1.43 Å)**



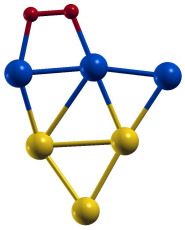
**$Au_1Pt_5$-7_2-C**

**(1.50 Å)**



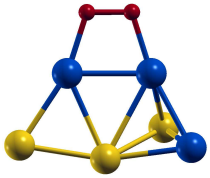
**$Au_2Pt_4$-GS_3-C**

**(1.29 Å)**



**$Au_3Pt_3$-GS_2-D**

**(1.35 Å)**

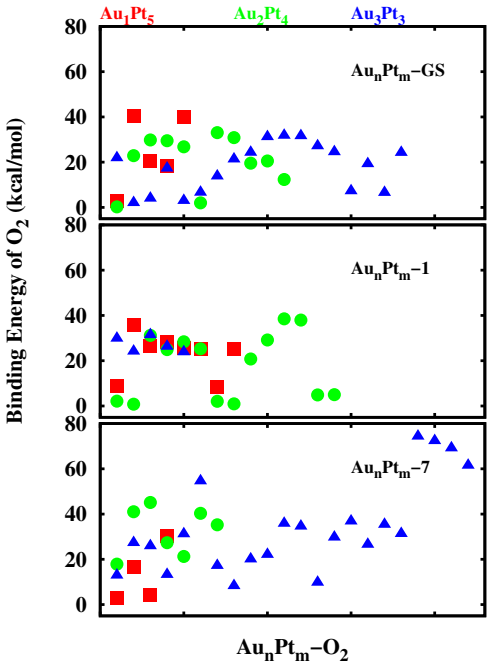


**$Au_3Pt_3$-7_2-B**

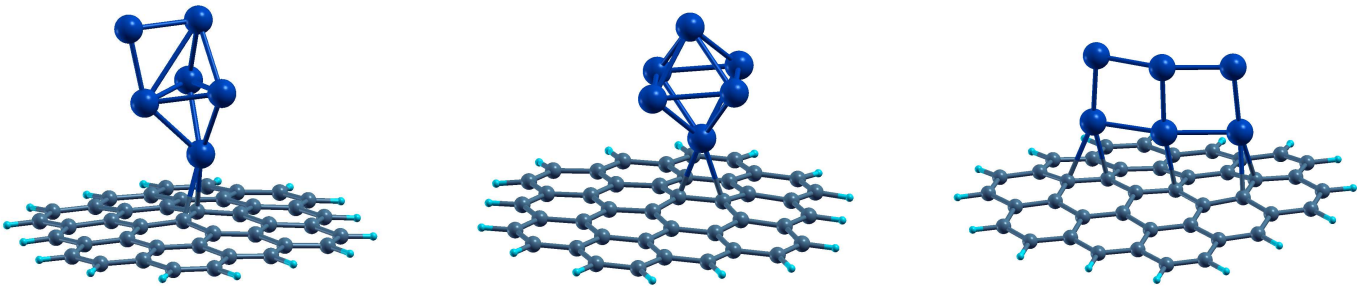
**(1.38 Å)**

Supp-Fig. 3

Geometries of $O_2$ adsorbed $Au_nPt_m$ clusters with enhanced O-O bond activation. The optimized O-O bond distance ($\mathring{A}$) in the complex is given in parenthesis (blue color).

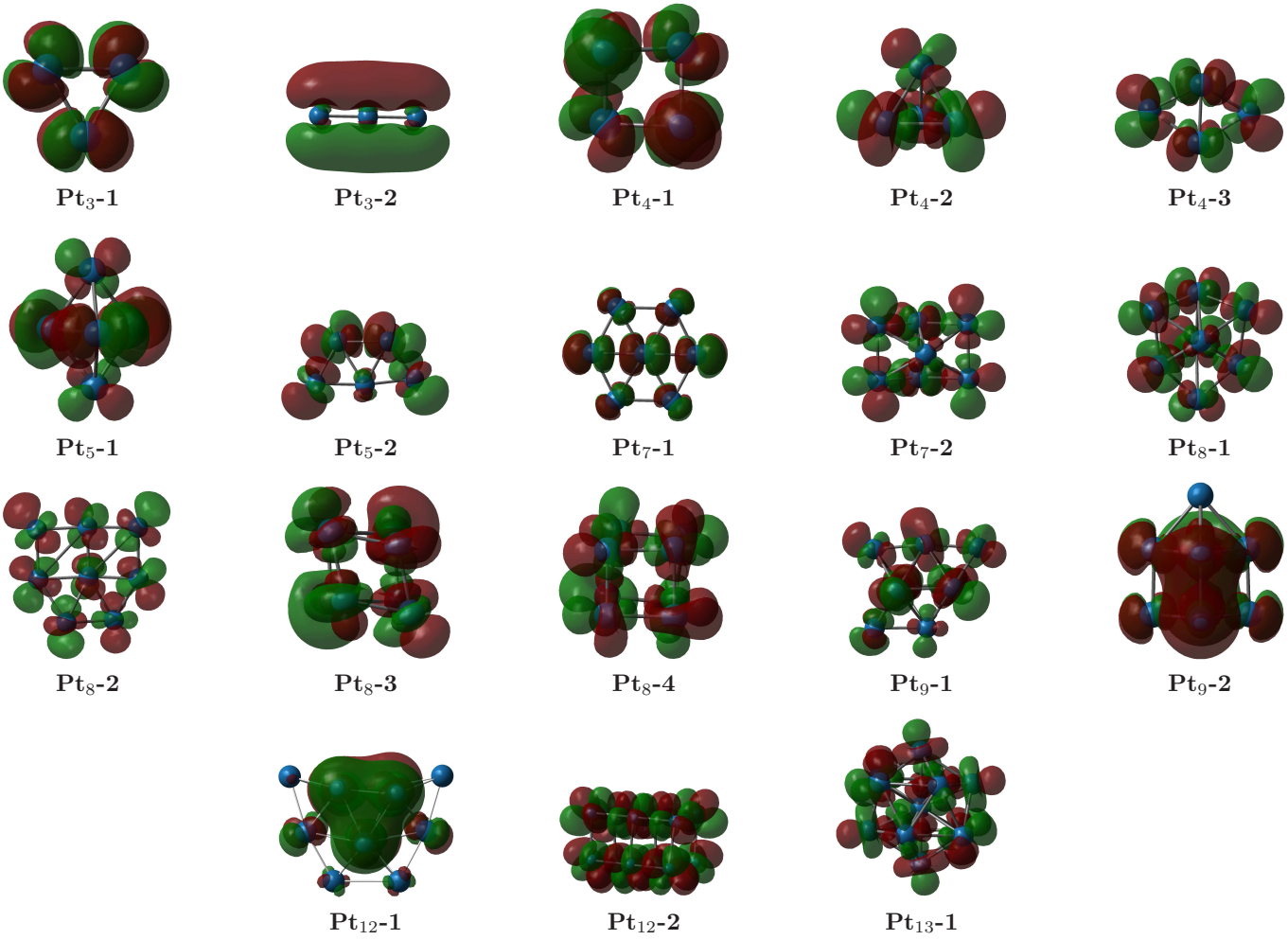



Supp-Fig. 4
Binding energy (kcal/mol) of $O_2$ with various $Au_nPt_m$ conformations. Red squares represent binding energies with $Au_1Pt_5$ conformations for each shape. Green spheres represent binding energies with $Au_2Pt_4$ conformations for each shape. Blue triangles represent binding energies with $Au_3Pt_3$ conformations for each shape.



**C42-Pt$_6$-1** **C42-Pt$_6$-2** **C42-Pt$_6$-7**

Supp-Fig. 5
Optimized $Pt_6$-m (m=1,2,7)–graphene nano flake ($C_{42}$ with zig-zag edges) complexes.




Supp-Fig. 6
HOMOs of $Pt_m$ clusters where, m = 3-13.