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Electronic Interaction between Platinum Nanoparticles and Nitrogen-doped Reduced Graphene Oxide: Effect on the Oxygen Reduction Reaction

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Supplementary Information

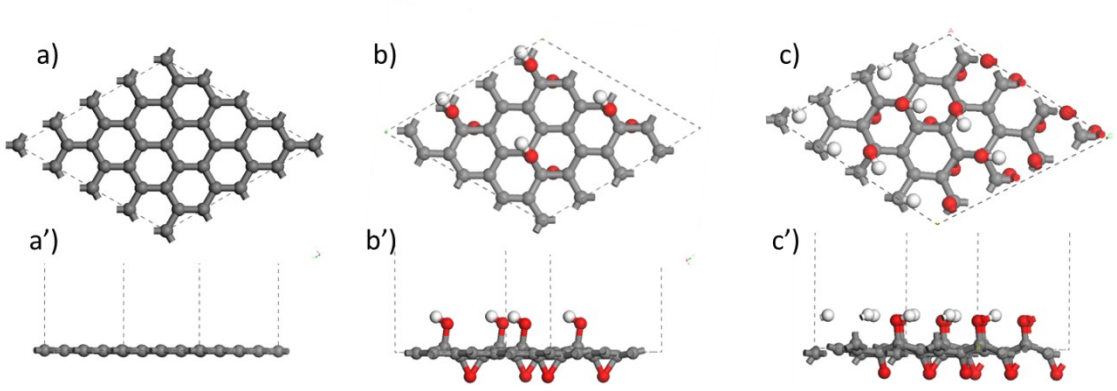

Figure S1. Top and side views of a) 4x4 graphene sheet, b) LOG and c) HOG.

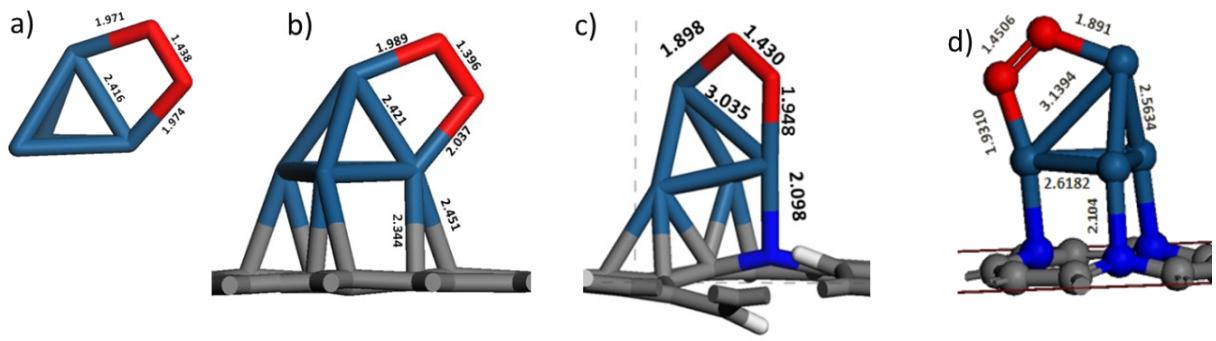

Figure S2. Interaction of molecular Oxygen with Pt_4 a) unsupported, b) Graphene supported, c) Graphene 1N doped and d) Graphene 3N doped. Pt-C distances shown after O_2 adsorption are larger than those previous to O_2 adsorption shown in Table 6.

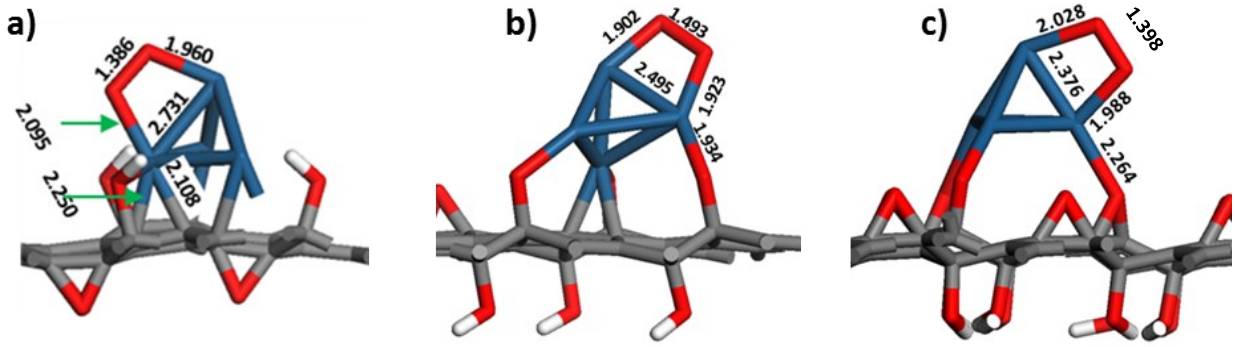

Figure S3. Interaction of molecular Oxygen with Pt_4 supported on a) LOG in the OH side, b) LOG in the epoxy side and c) HOG in the epoxy side.

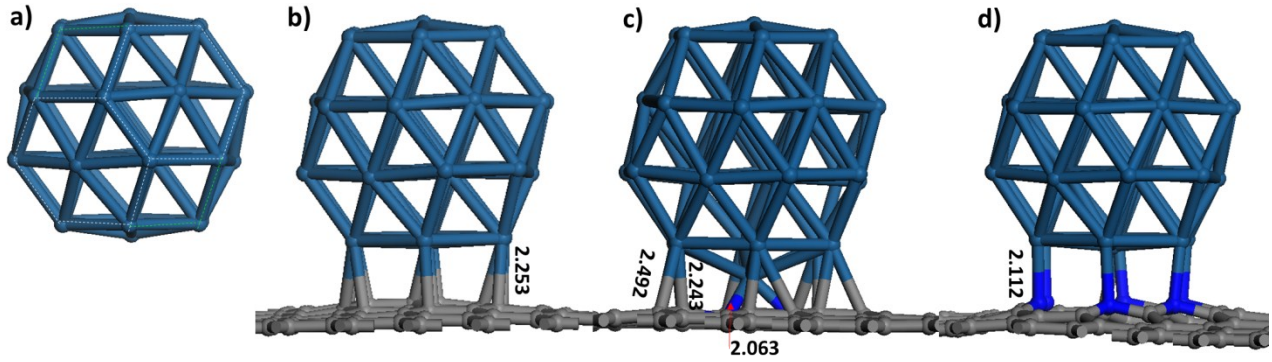

Figure S4. Pt_{38} clusters interacting with the support; a) unsupported, b) supported on graphene, c) supported on G-3N and d) supported on G-6N.

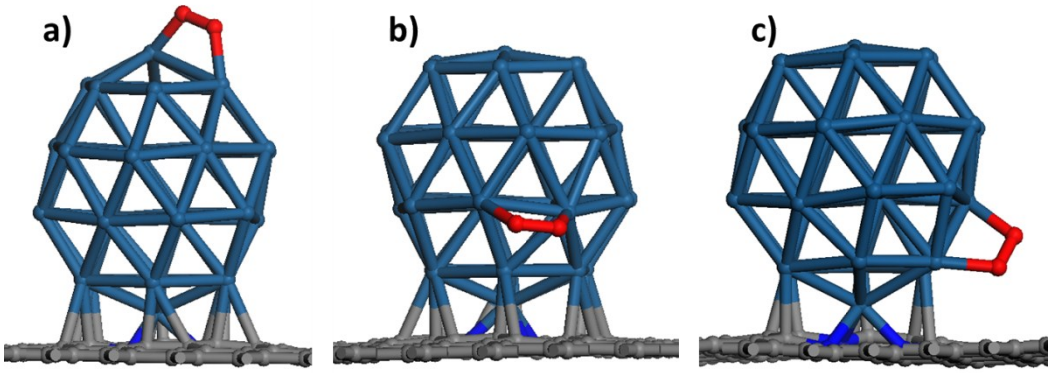

Figure S5. Position of molecular oxygen interacting with the Pt_{38} cluster supported in N3-doped graphene. a) top position, b) middle position and c) interface position.

Table S1. Calculated lattice parameters (LP) and Bader electronic charges of the supports in this study. Parenthesis values represent Bader charges per atom or functional group.

	LP / Å	Bader Charges (e)			
		G	O	OH	N
Graphene	9.87	0.0 (±0.1)			
LOG	9.98	5.05 (±0.07)	-3.14 (-0.79)	-1.91 (-0.48)	
HOG	10.01	10.4 (±0.06)	-6.57 (-0.82)	-3.87 (-0.48)	
G-1N	9.87	1.22 (±0.1)			-1.22
LOG-1N	9.98	6.29 (±0.09)	-3.15 (-0.79)	-1.90 (-0.48)	-1.24
HOG-1N	10.01	11.5 (±1.1)	-7.73 (-0.97)	-2.77 (-0.34)	-0.95
G-3N	9.858	3.20 (±0.1)			-3.20

Table S2. DFT calculated lattice parameter (LP) and overall electronic charge of the support before and after deposition of Pt_{38} over the support. Two values of interaction energy between cluster and support (E_{int}) are reported in each case separated by a slash: the first was calculated without considering deformation of cluster and support and the second includes such deformation effect.

	Support			Pt_{38}-Over Support			
	LP (Å)	Charge (e)		E_{int} (eV)	Charge (e)		
		G	N		G	N	Pt
Pt_{38}					-	-	0.0
C6x6	17.281	0	-	0.07/-1.38	0.084		-0.084
C6x6-3N	17.273	+3.62	-3.62	-1.51/-3.93	2.75	-2.96	0.16
C6x6-6N	17.243	+6.83	-6.83	-3.23/-4.6	5.68	-6.15	0.48