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Supplementary Information

Effect of Graphene with Nanopore on Metal Clusters Properties

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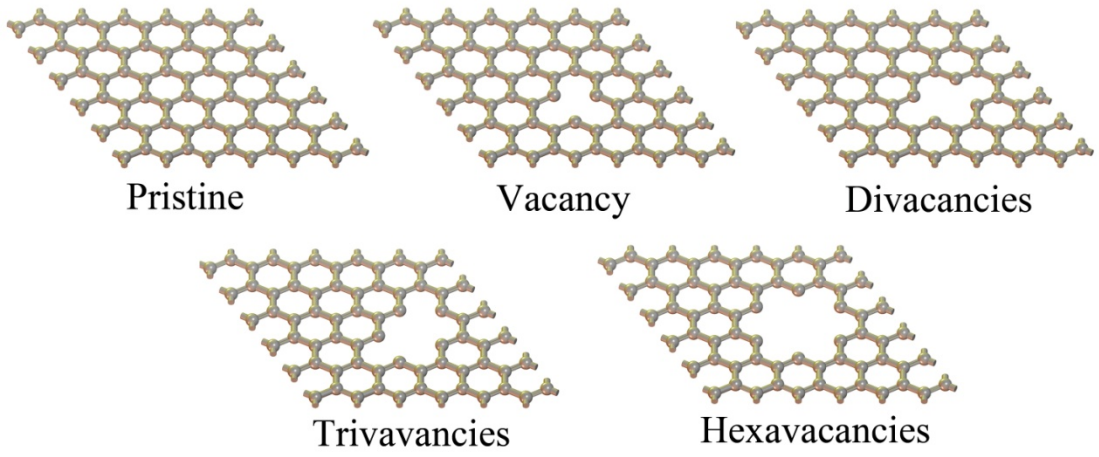


Figure S1. Pristine graphene and graphene with different size nanopore

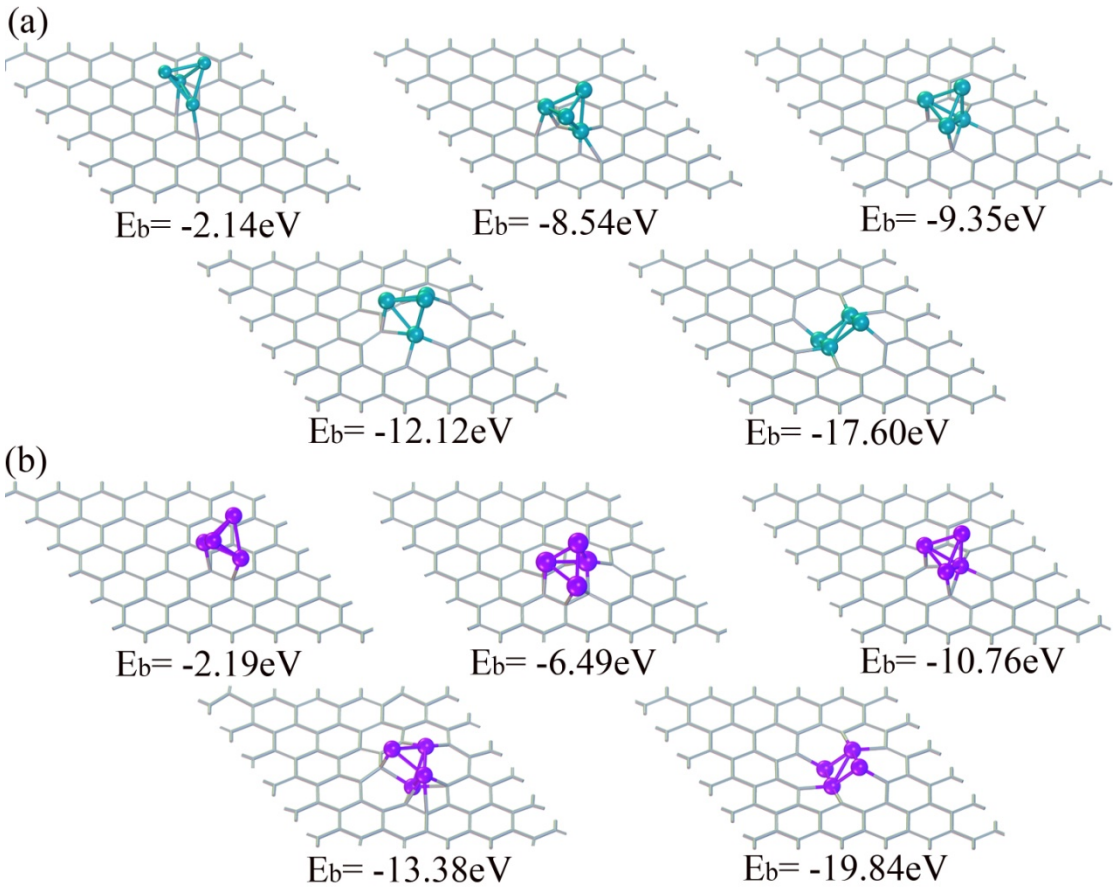
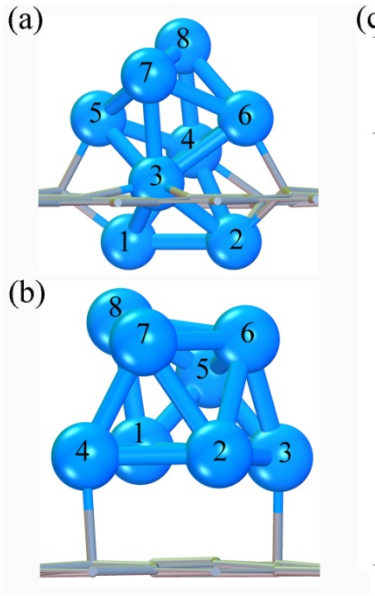


Figure S2. Optimized structures and binding energies of (a) Rh_4, (b) Ir_4 on different graphene (G, GV, GV1, GV2, GV3, GV6).



(c)

Atoms	Charge (e)	
	Pd (GV6)	Pd (G)
1	0.23	0.12
2	0.22	0.12
3	0.21	0.10
4	0.20	0.11
5	0.12	-0.02
6	0.12	0.00
7	0.12	-0.02
8	0.02	0.01
Total	**1.24**	**0.42**

Figure S3. Charge of each Pd atoms on hexavacancies and pristine graphene (a), (b) relevant Pd atoms (c) charge of relevant Pd atoms.

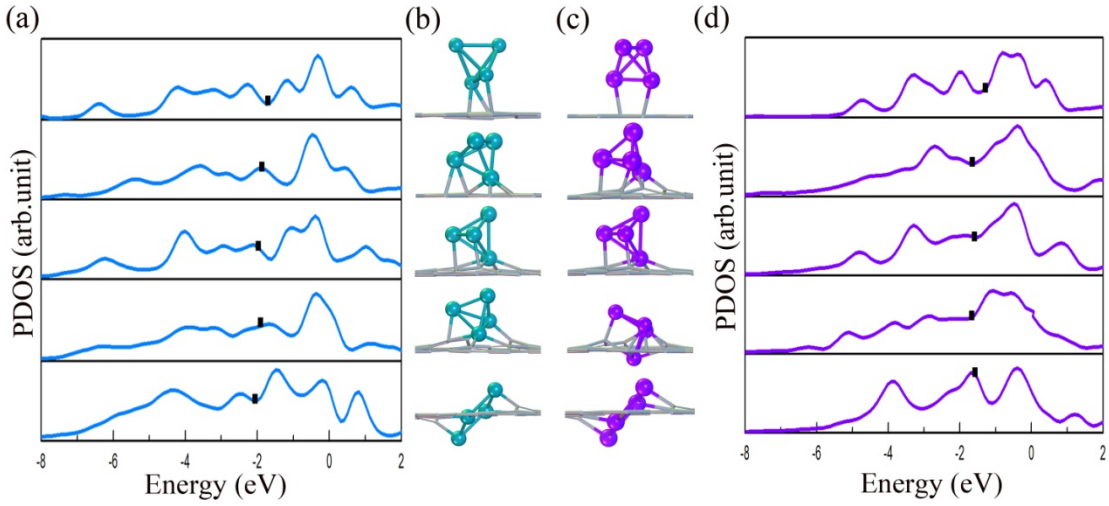


Figure S4. Projected density of states(PDOS) of the most stable adsorption structures on each graphene support (G, GV1, GV2, GV3, GV6). (a) PDOS of Ir_4 clusters, (b) relevant Ir_4-Graphene structures, (c) relevant Rh4-Graphene structures, (d). PDOS of Rh_4 clusters.

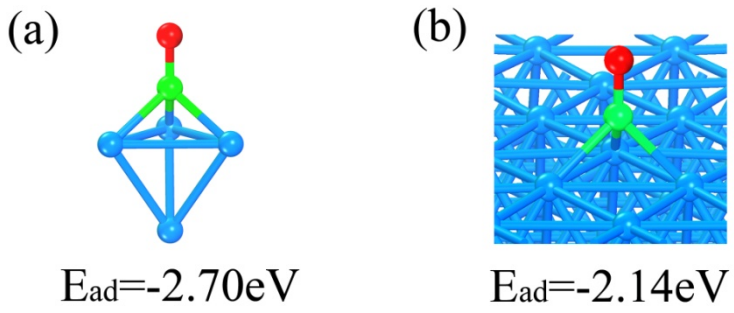


Figure S5. Optimized structures and CO adsorption energies on (a) Pd_4, (b) Pd_{111}.