Electronic Supplementary Material (ESI) for Nanoscale.

Crowned graphene: from coordination chemistry on graphene to graphitic carbon oxide

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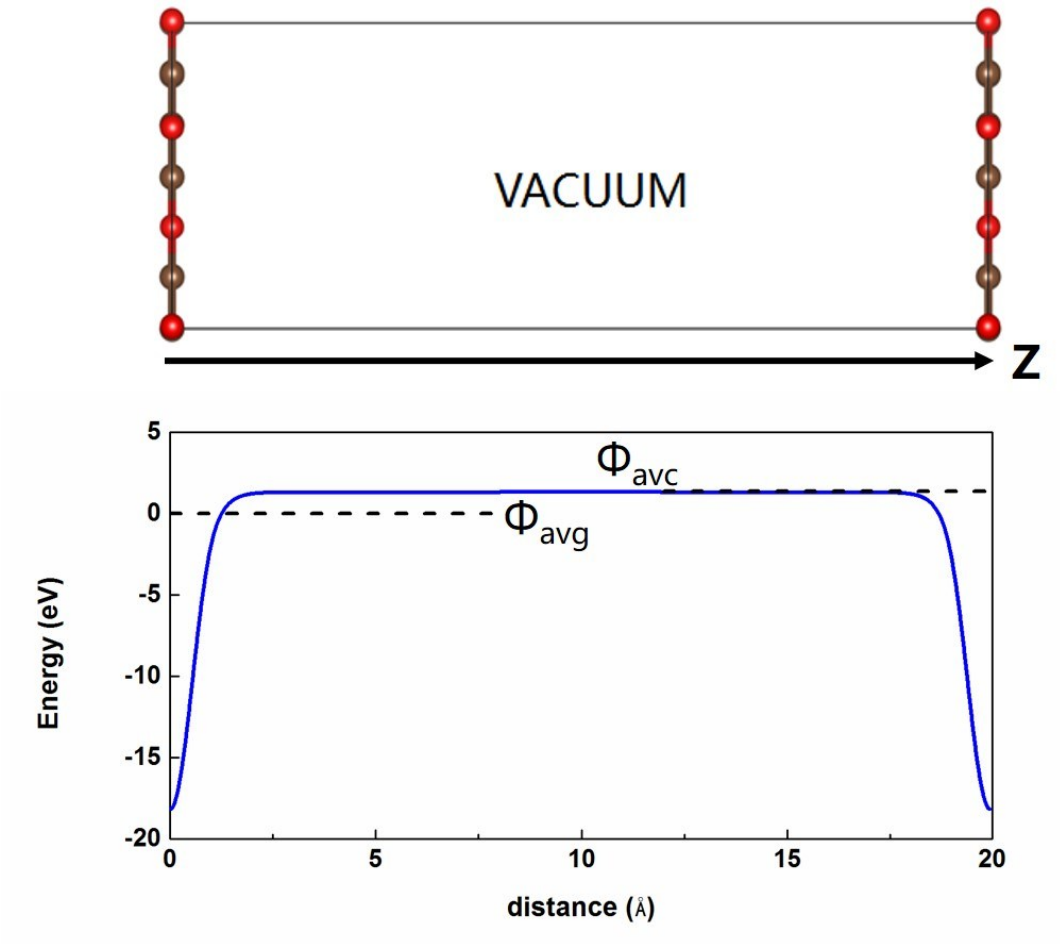
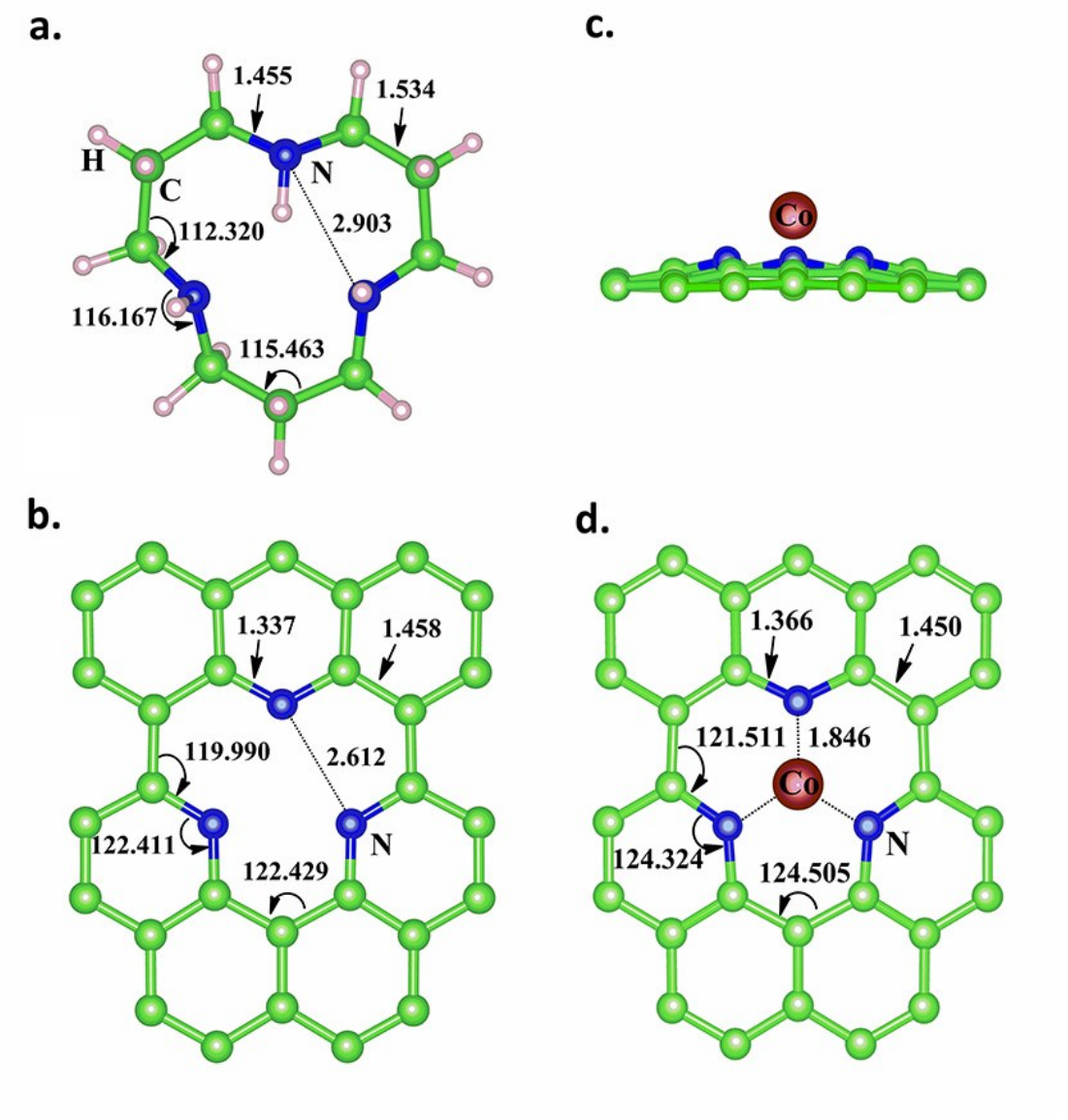
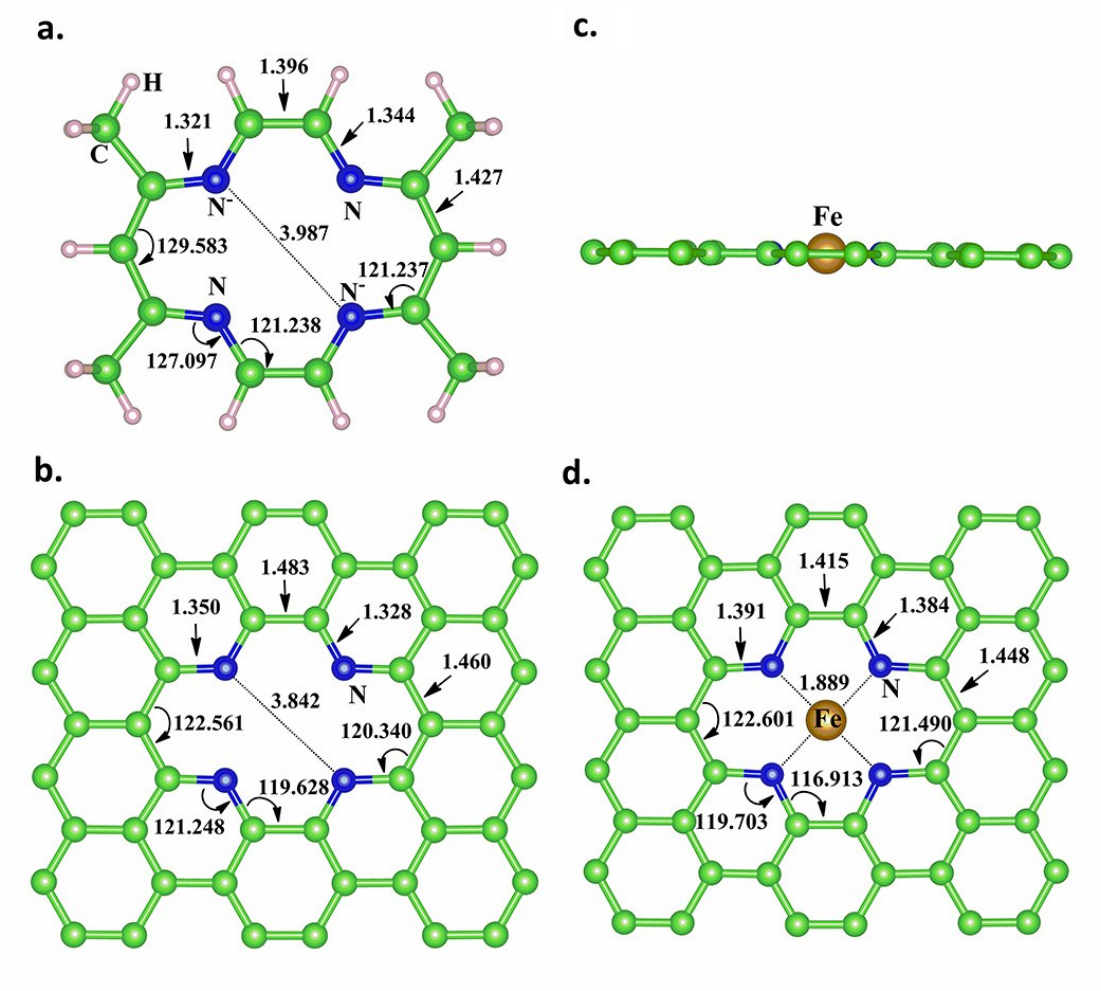


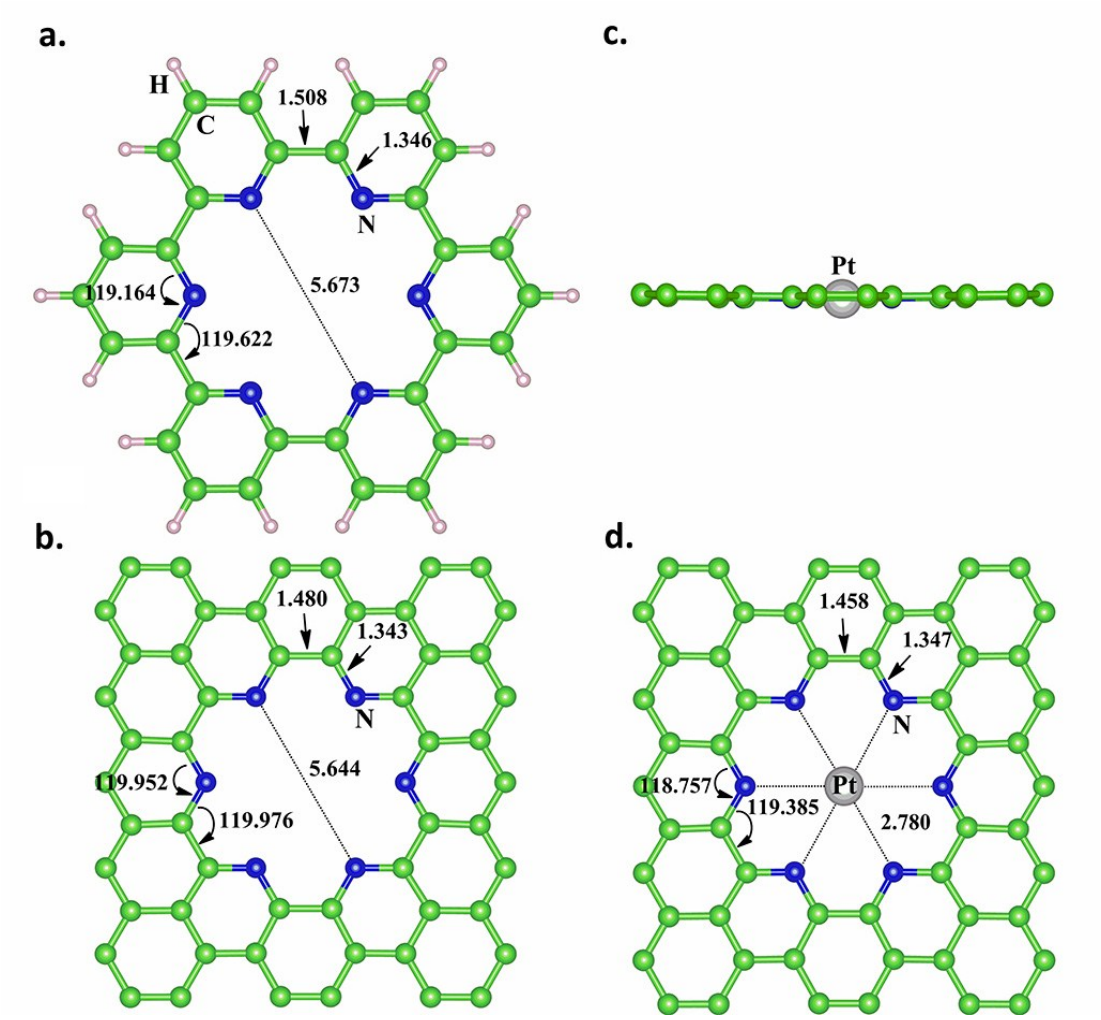
Supplementary Figure S1. A schematic model (top) and the corresponding profile of the calculated electrostatic potential (bottom). The dashed lines show the average electrostatic potential (Φ_{avg}) and the electrostatic potential at the center of the vacuum region (Φ_{avc}).



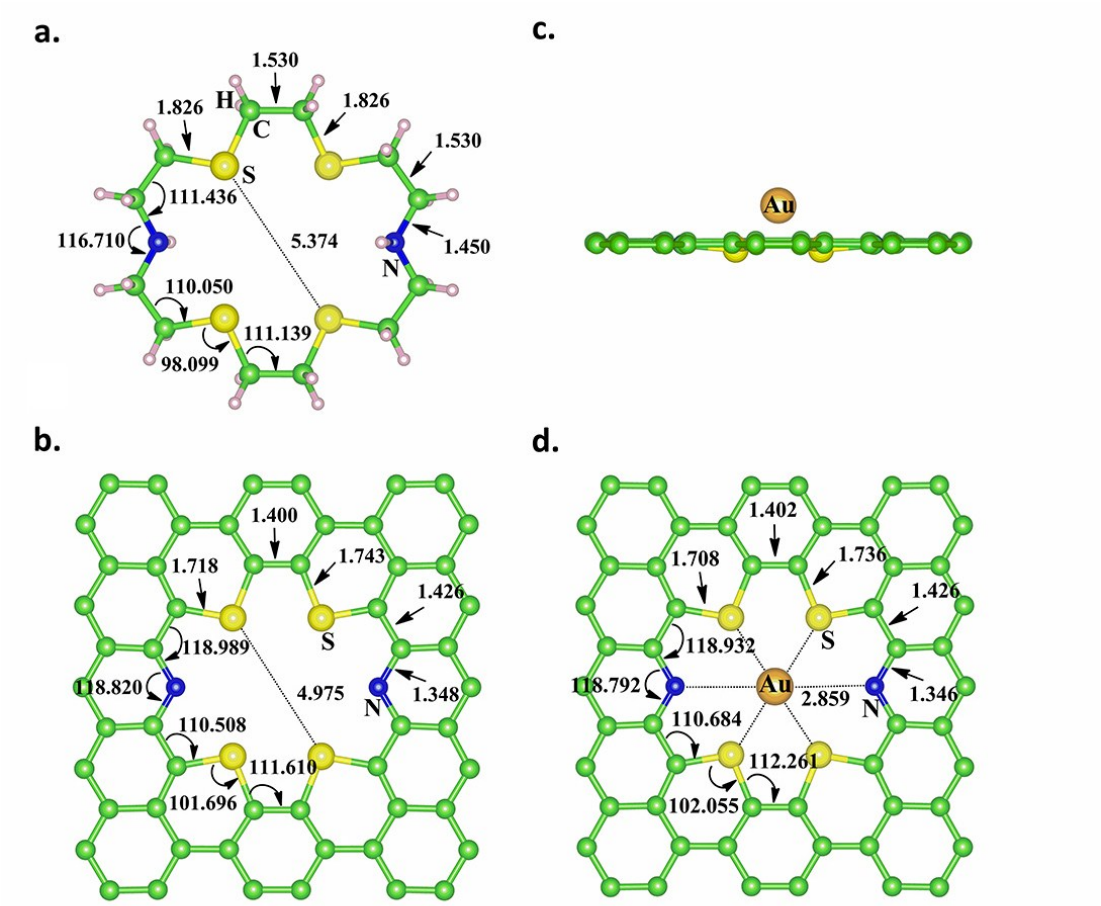
Supplementary Figure S2. a. Structure and parameters of 1,5,9-triazacyclododecane; **b.** structure and parameters of 1,5,9-triazacyclododecane embedded in graphene; **c. and d.** the top and side view of Co adsorbed at the triazacyclododecane site.



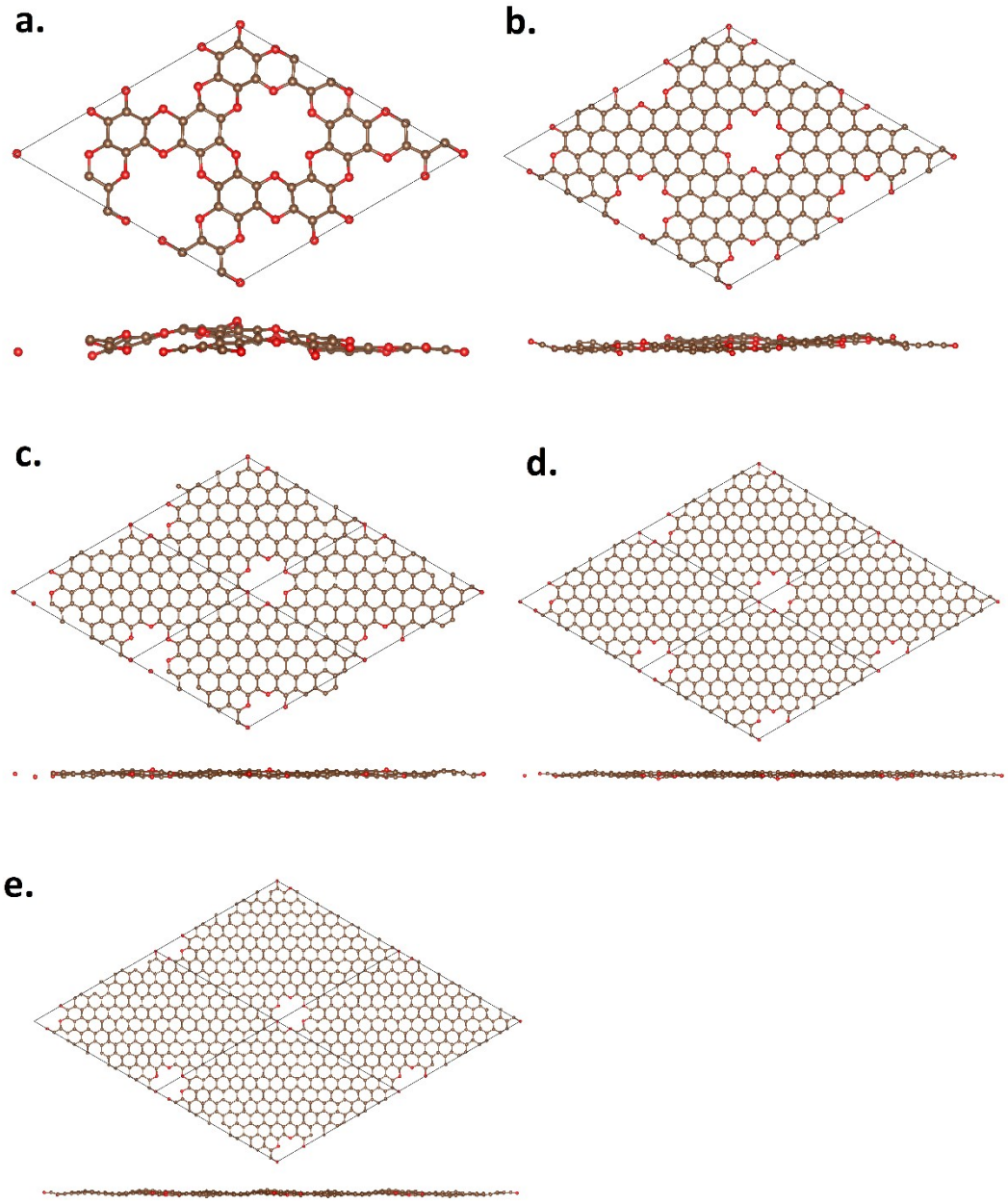
Supplementary Figure S3. a. Structure and parameters of 5,7,12,14-tetramethyl-1,4,8,11-tetraazacyclotetradecane; **b.** structure and parameters of 5,7,12,14-tetramethyl-1,4,8,11-tetraazacyclotetradecane embedded in graphene; **c. and d.** the top and side view of Fe adsorbed at the tetraazacyclotetradecane site.



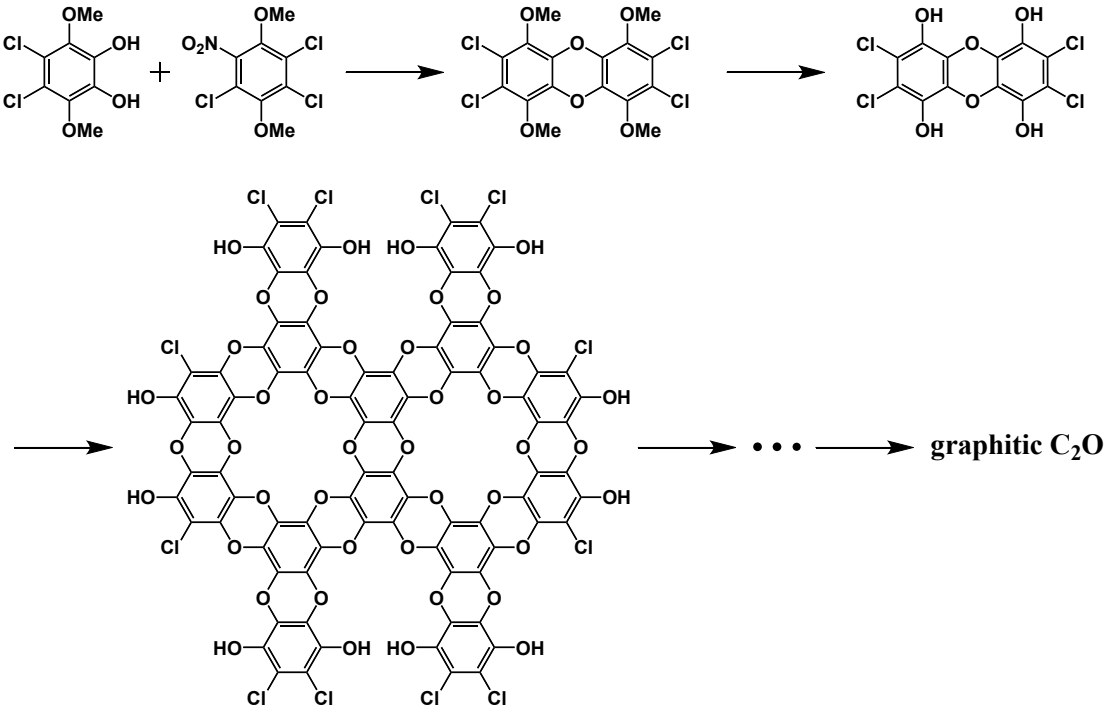
Supplementary Figure S4. a. Structure and parameters of cyclohexapyridine; **b.** structure and parameters of cyclohexapyridine embedded in graphene; **c. and d.** the top and side view of Pt adsorbed at the cyclohexapyridine site.



Supplementary Figure S5. a. Structure and parameters of 1,4,10,13-tetrathia-7,16-diazacyclooctadecane; **b.** structure and parameters of 1,4,10,13-tetrathia-7,16-diazacyclooctadecane embedded in graphene; **c. and d.** the top and side view of Au adsorbed at the 1,4,10,13-tetrathia-7,16-diazacyclooctadecane site.



Supplementary Figure S6. A snapshot of the equilibrium structure of **a.** 2-CG; **b.** 3-CG; **c.** 4-CG; **d.** 5-CG; **e.** 6-CG, respectively, after 5ps MD simulation at 1000 K.



Supplementary Scheme S1. The designed synthetic route to prepare graphitic C_2O from small molecules.