

Supplementary Information

On the Use of Graphene Nanosheets for the Drug Delivery: A Case Study of Cisplatin and some of its Analogs

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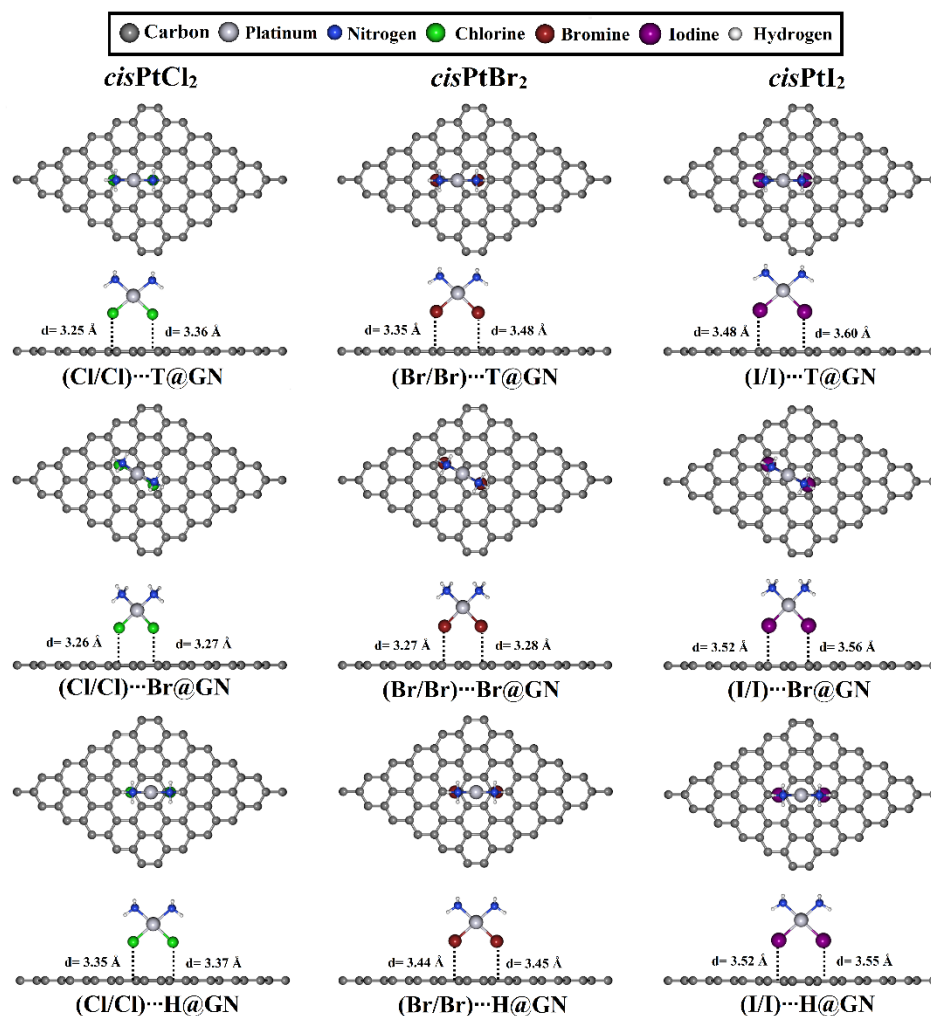


Figure S1. Top and side views of all the relaxed structures for *cis*PtX₂...GN complexes (where X = Cl, Br, and I) in perpendicular and parallel configurations at all adsorption sites. The equilibrium distances (d) are presented in Å.

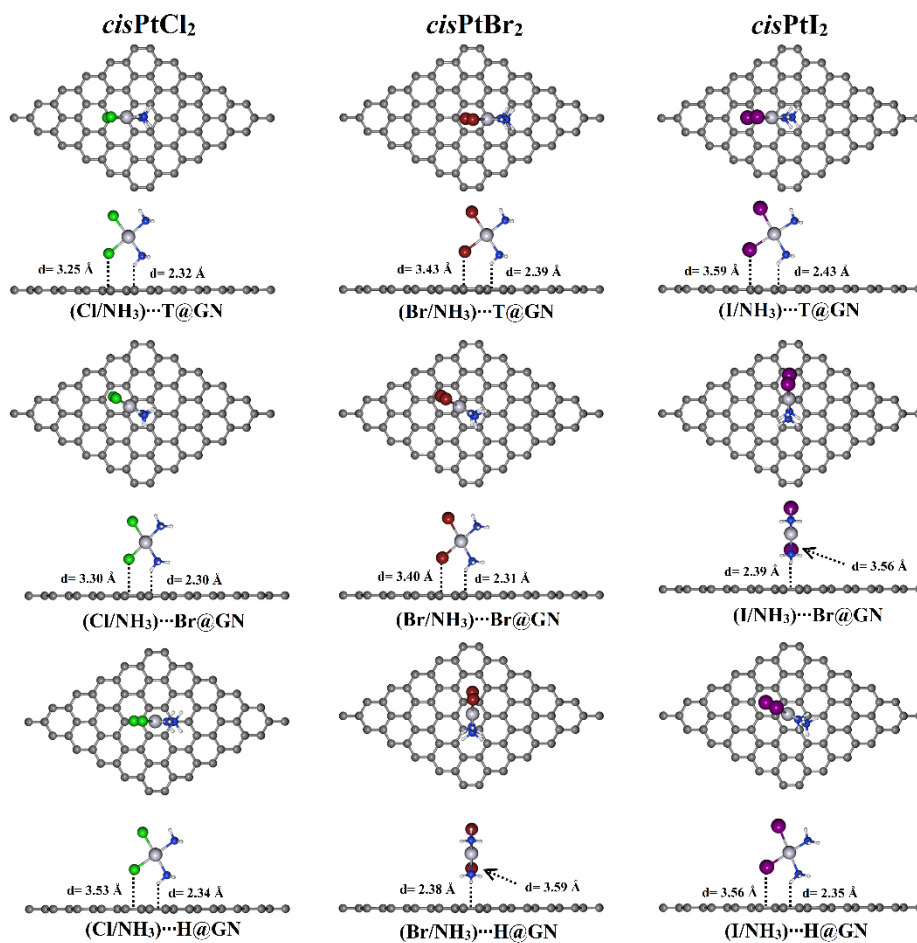
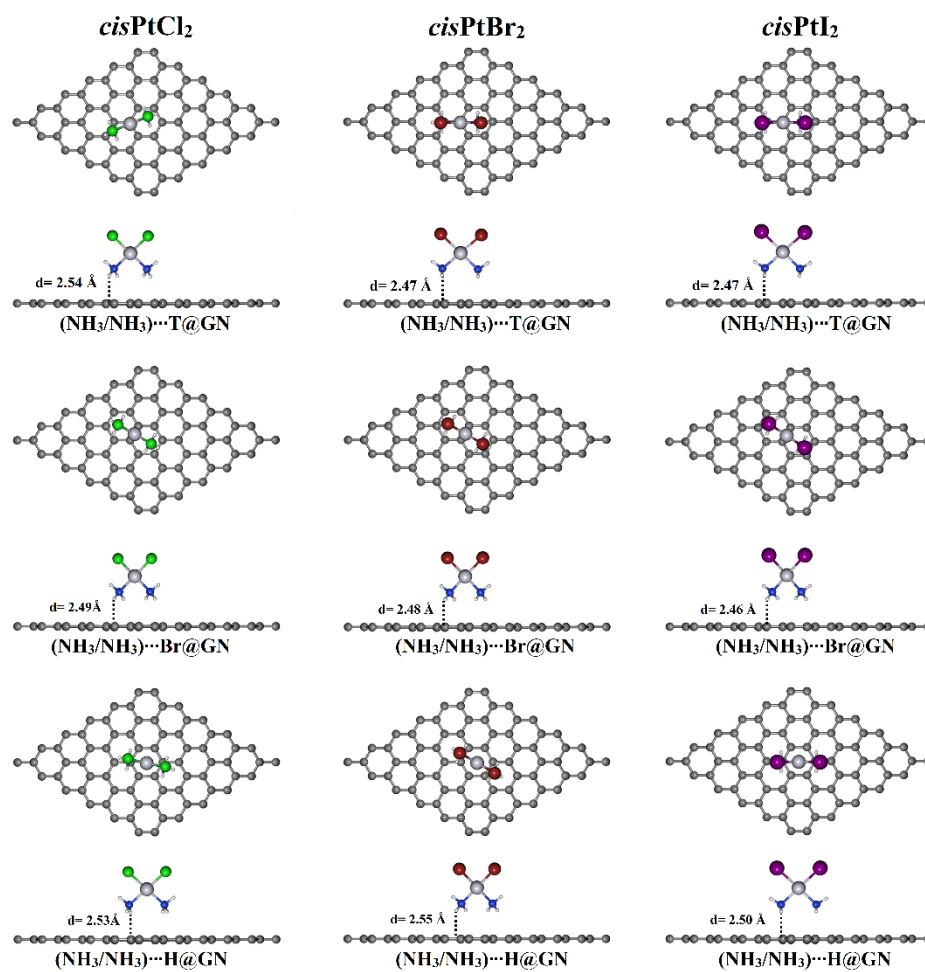


Figure S1. Continued.

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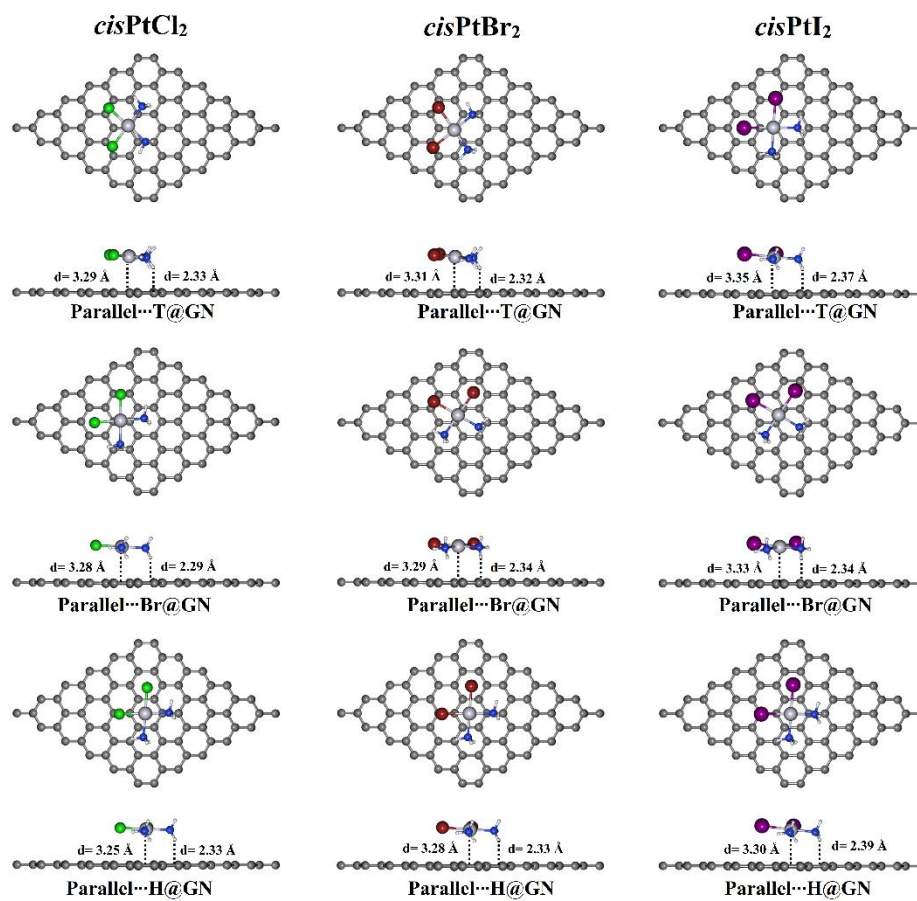


Figure S1. Continued.

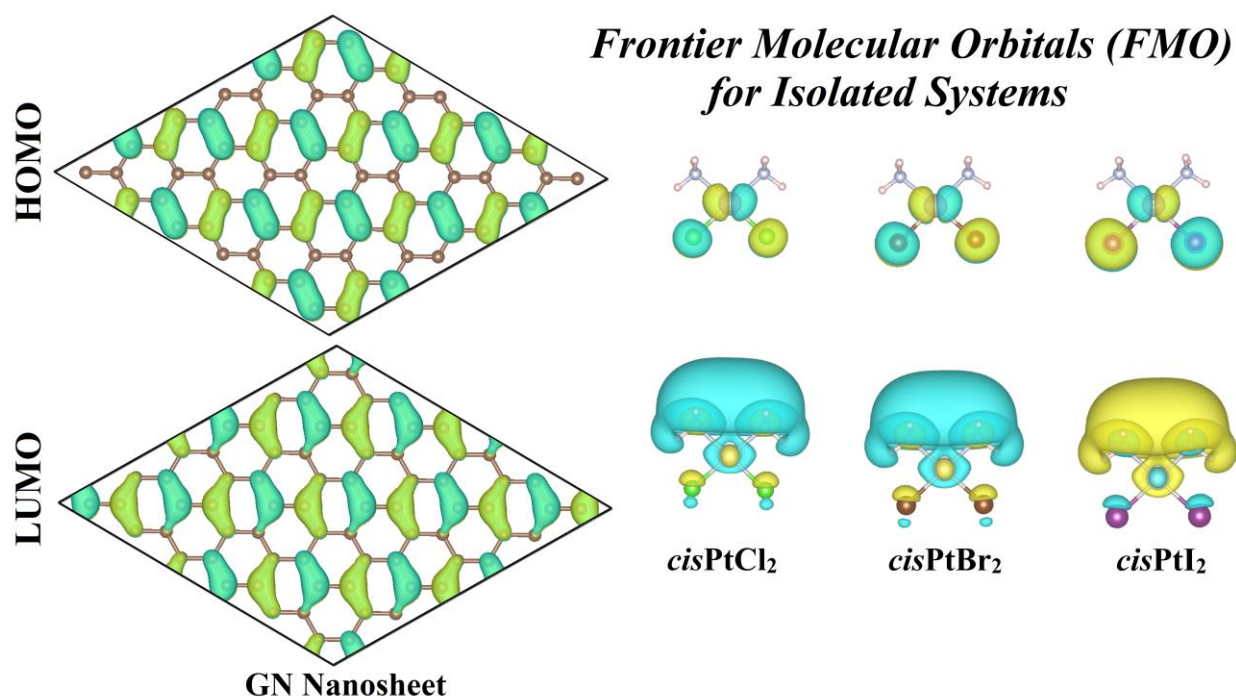


Figure S2. Distributions of HOMO and LUMO for the GN nanosheet and *cisPtX₂* molecules before the adsorption process. Pale brown, silver, pink, gray, green, dark brown, and violet balls refer to carbon, platinum, hydrogen, nitrogen, chloride, bromide, and iodide atoms, respectively.

Frontier Molecular Orbitals (FMO)

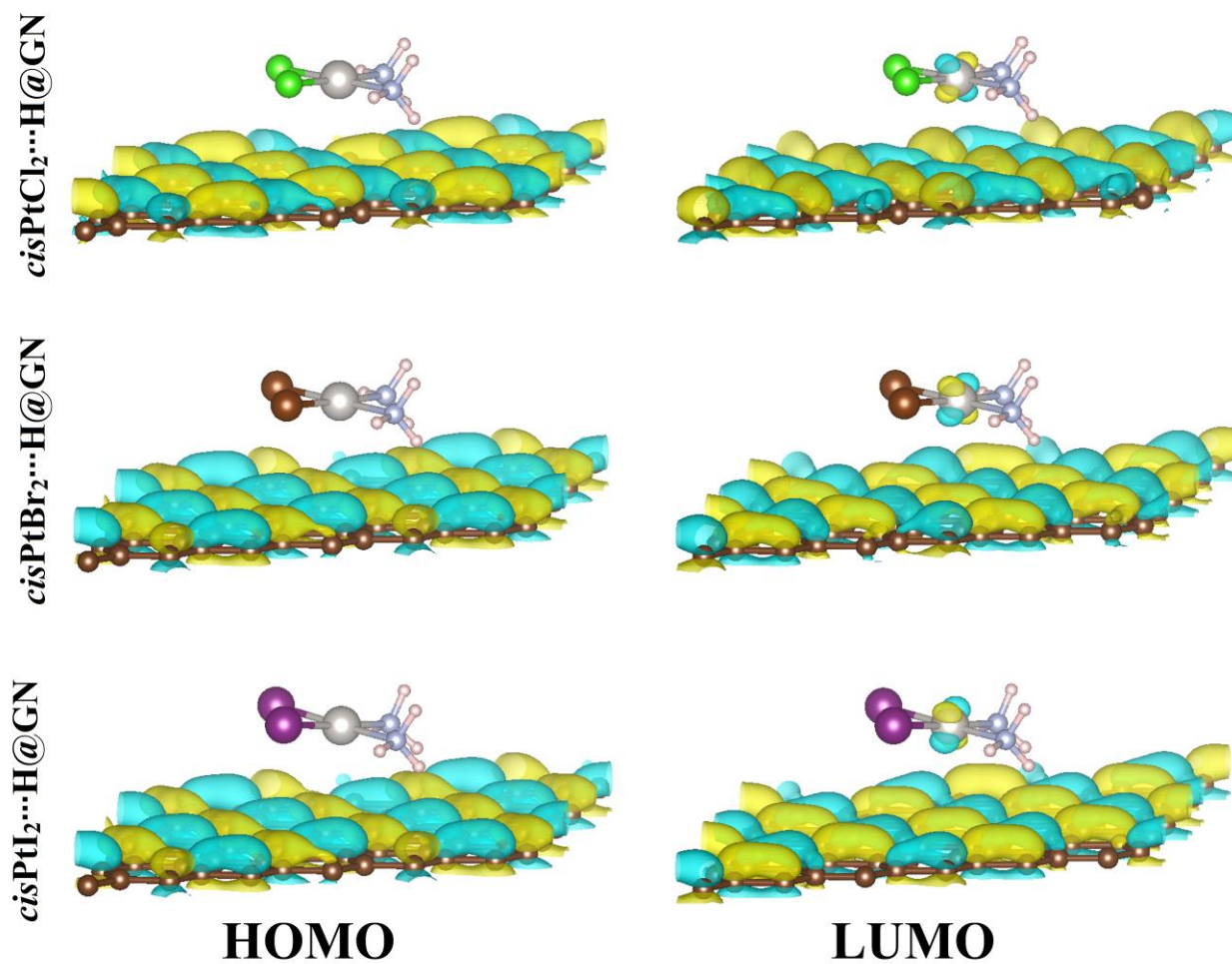


Figure S3. Distributions of HOMO and LUMO for the most favorable relaxed $cisPtX_2 \cdots GN$ complexes within the parallel configuration. Pale brown, silver, pink, gray, green, dark brown, and violet balls refer to carbon, platinum, hydrogen, nitrogen, chloride, bromide, and iodide atoms, respectively.

Pristine Graphene (GN)

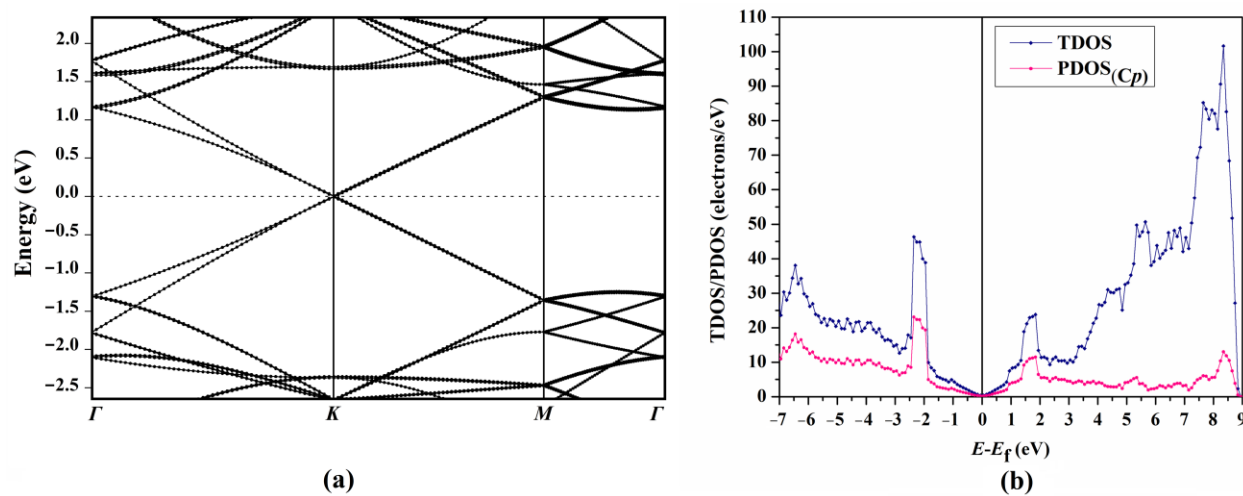


Figure S4. (a) Band structure of the pure GN nanosheet along high symmetry points of Brillouin zone, (b) Total and projected density of state (TDOS/PDOS) for the pure GN nanosheet, the contribution of p -orbital for carbon atom displayed by C_p . the Fermi level is located at zero energy.