Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Understanding the Non-covalent interaction mediated modulations to the electronic structure of quasi-zero-dimensional graphene nanoflakes

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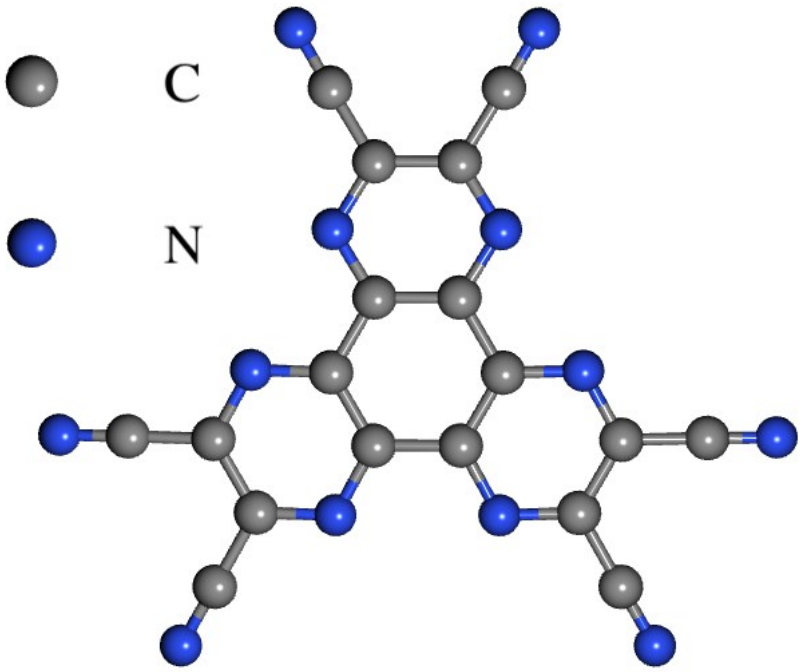

Figure S1: Pictorial representation of the hexaazatriphenylene-hexacarbonitrile (HATCN) molecule.

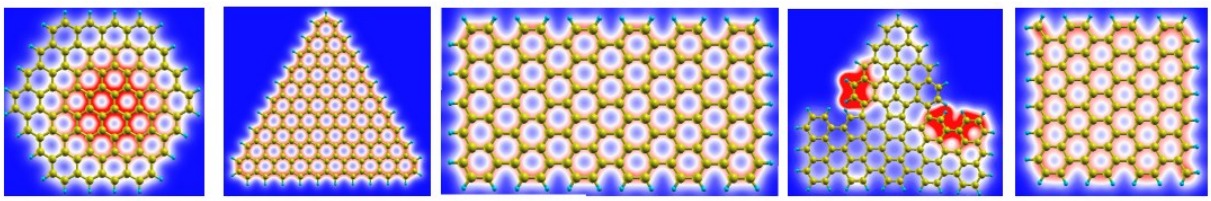

Figure S2: Computed 2D charge density distribution contour maps for the five GNF systems. Here the red and blue zones represent the gradual decrease in the electronic densities.

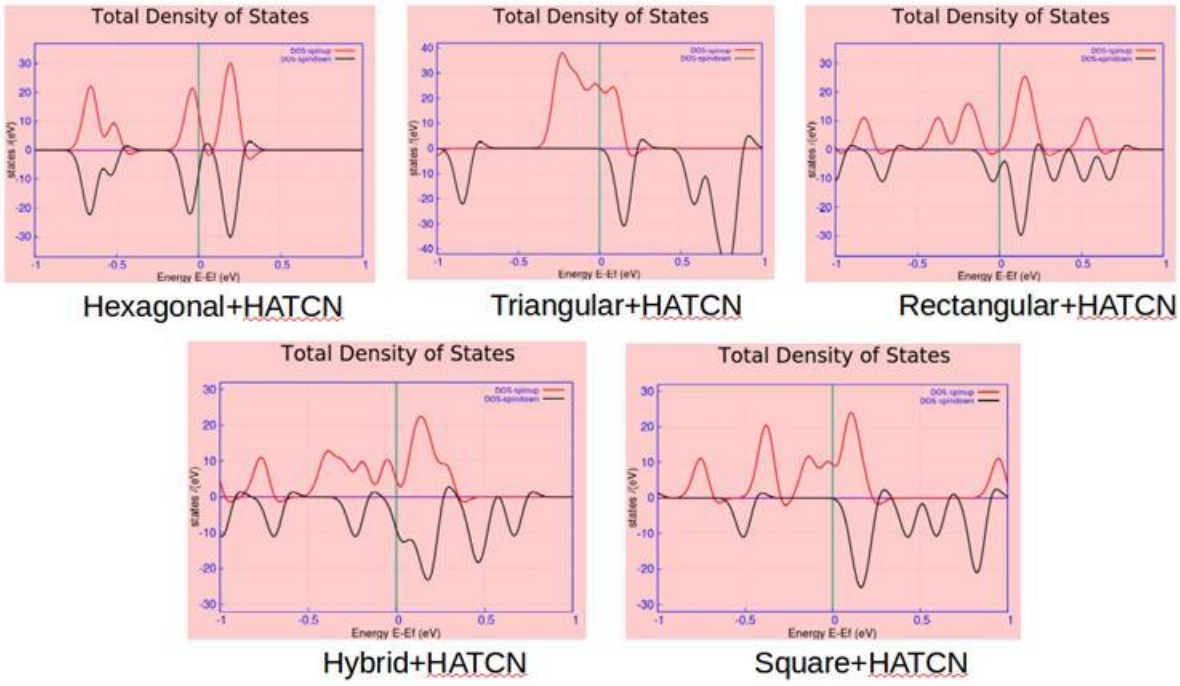

Figure S3: The graphical representations of the computed density of states (DOS) for the five different GNF-HATCN nanosystems. Here, the Fermi level is sets at zero.

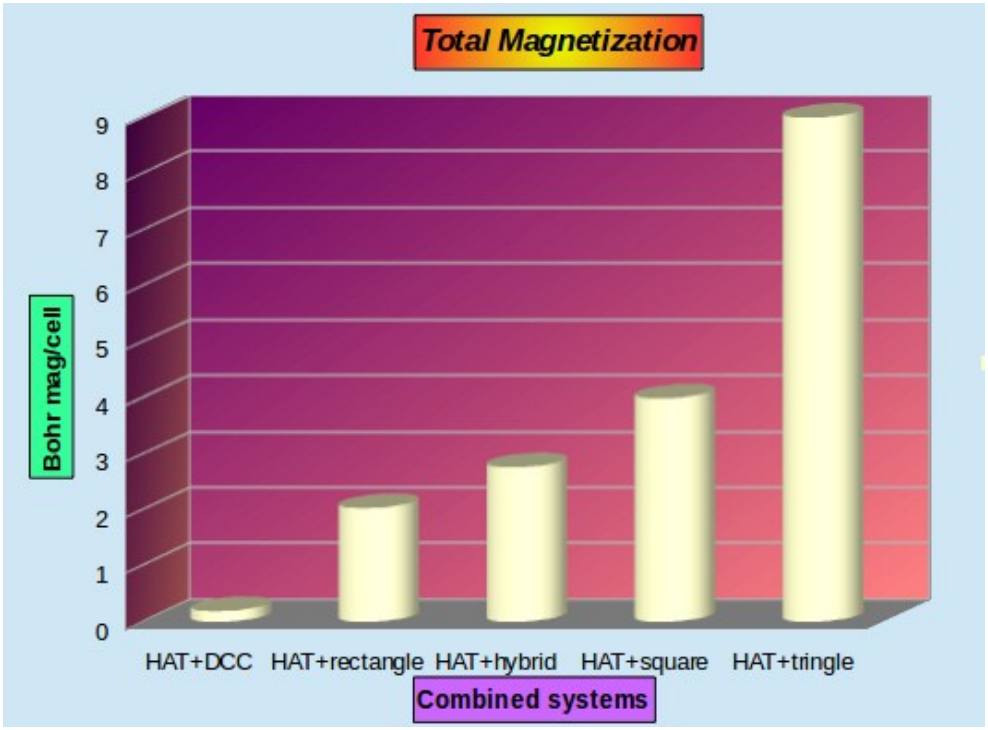

Figure S4: Computed total magnetization values for the five GNF-HATCN composite systems.

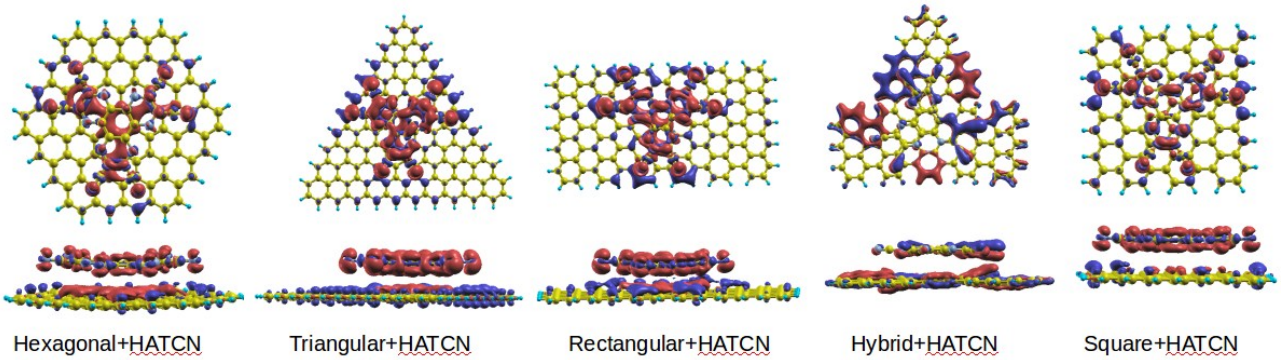

Figure S5: Computed differential charge density (DCD) distribution maps for the five GNF-HATCN combined systems. Here the red and blue zones represent the gradual increase and decrease in the electronic charges, respectively.