

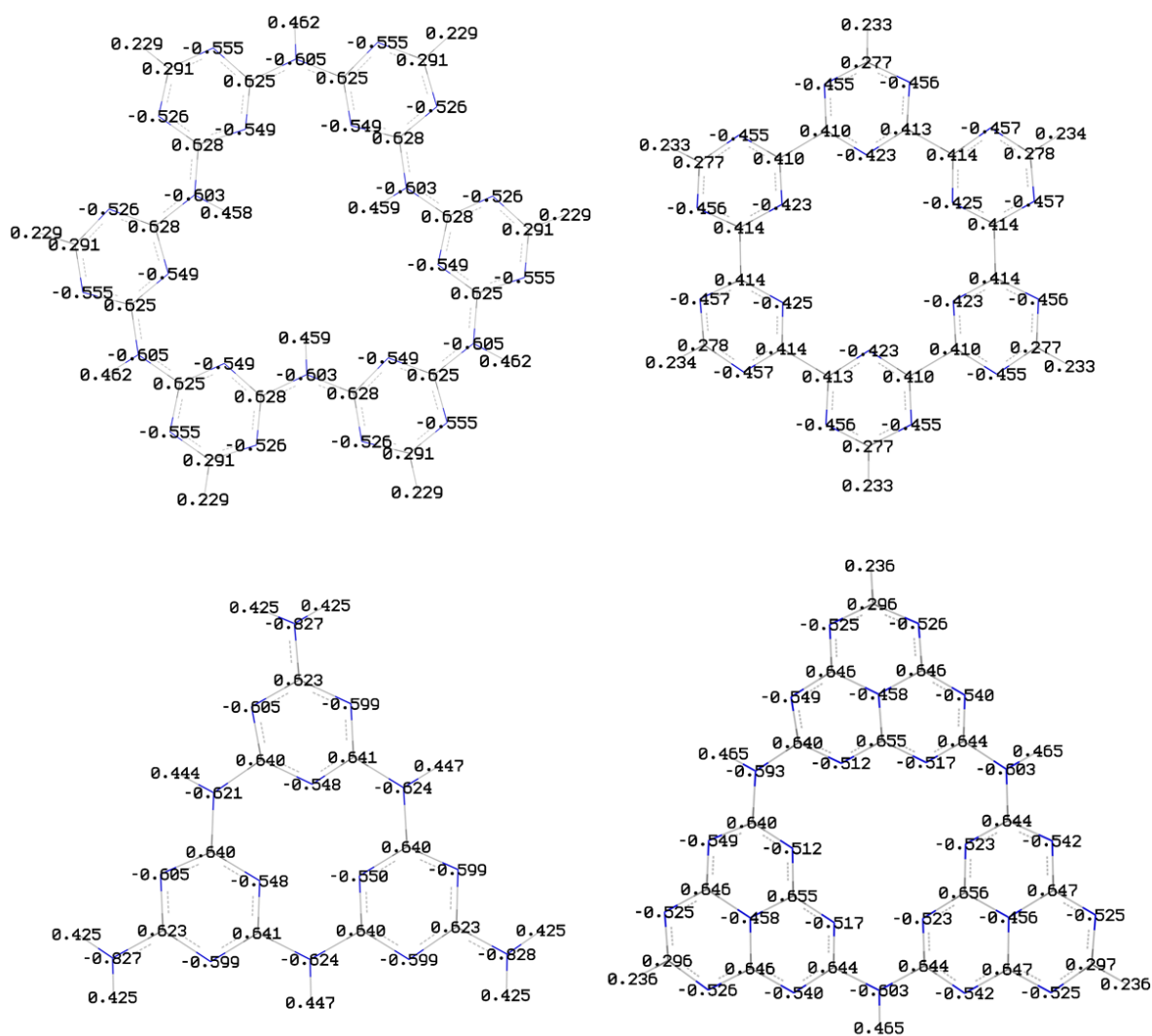
# Quantum chemical insights into porous s-triazine and tri-s-triazine carbon nitrides

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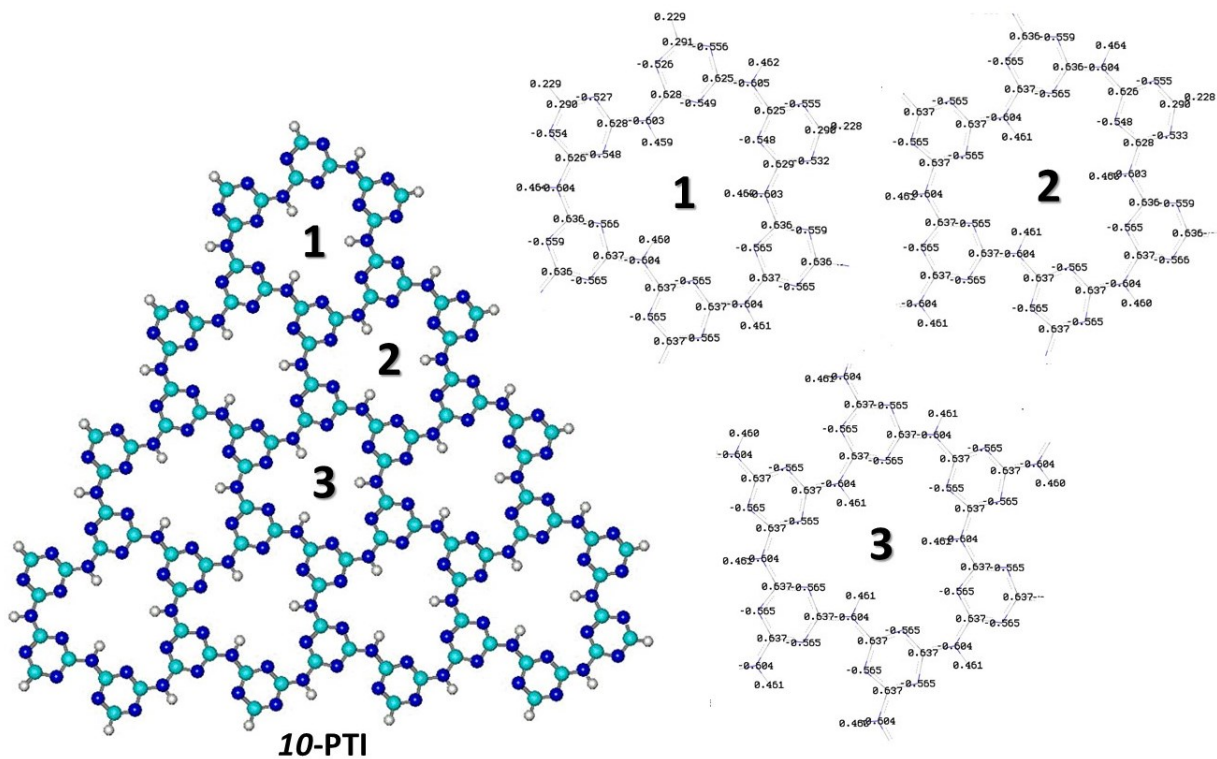
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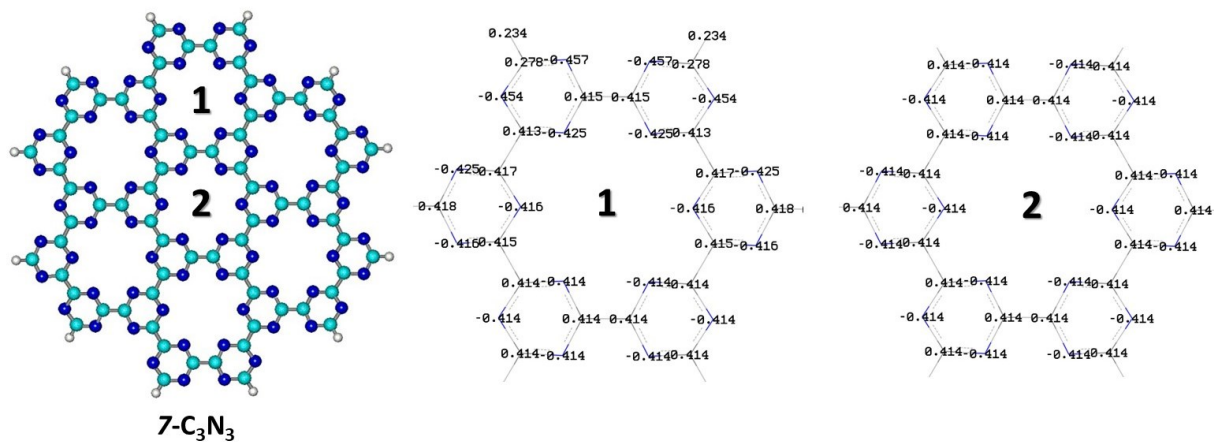
## Supporting Information



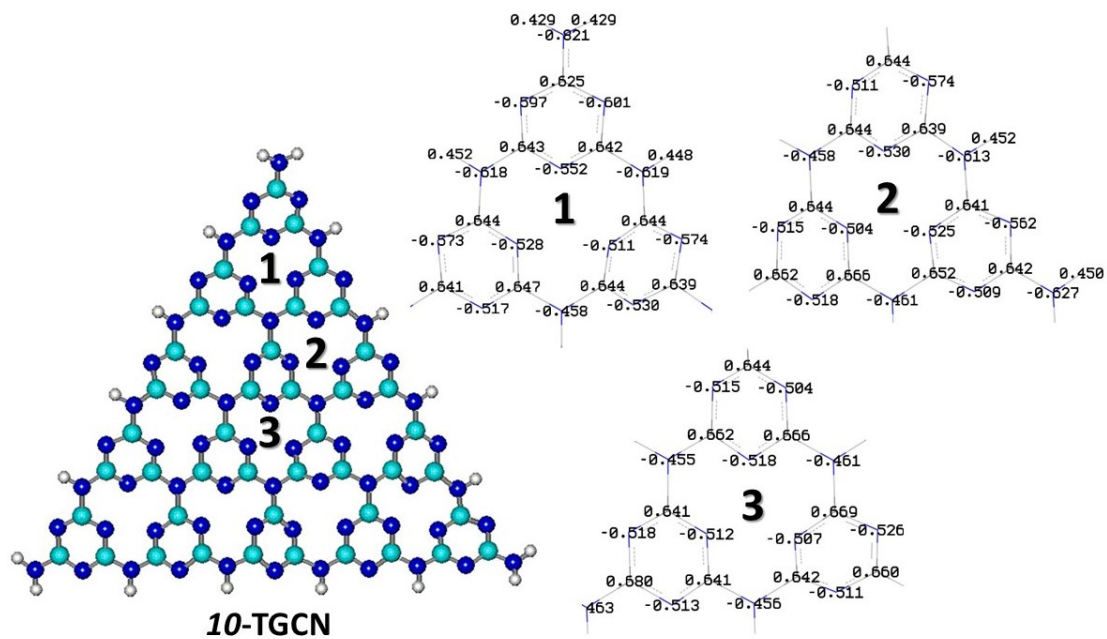
**Figure S1.** Atomic charges in single-pore models of PTI (top, left), C<sub>3</sub>N<sub>3</sub> (top, right), TGCN (bottom, left) and HGCN (bottom, right). The charges are calculated using the NBO scheme.



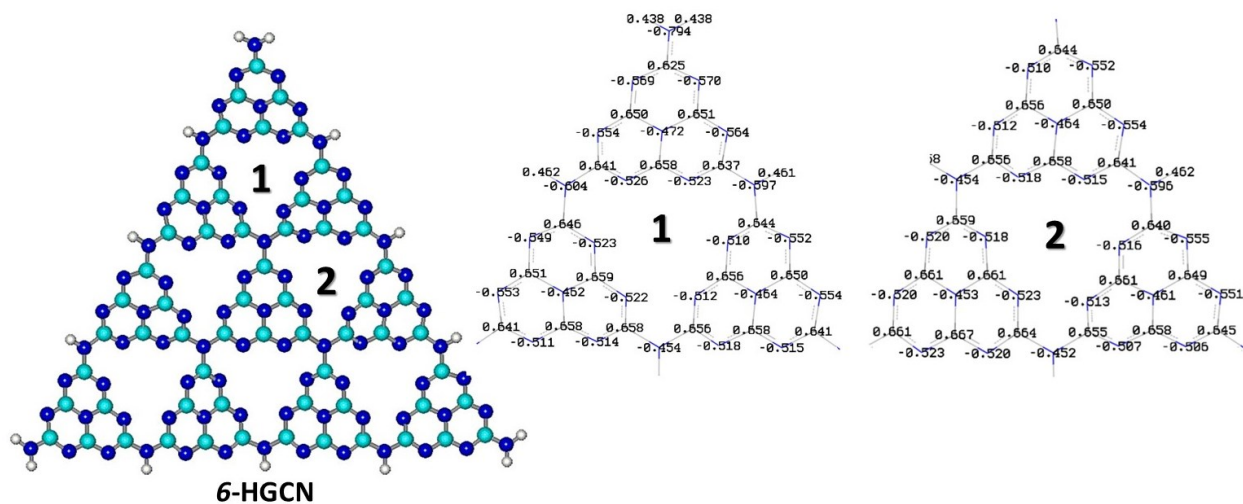
**Figure S2.** Representative atomic charges (for the pores numbered as 1, 2 and 3) in the PTI model with 10 nanopores. The charges are calculated using the NBO scheme.



**Figure S3.** Representative atomic charges (for the pore numbered as 1 and 2) in C<sub>3</sub>N<sub>3</sub> model with 7 nanopores. The charges are calculated using the NBO scheme.



**Figure S4.** Representative atomic charges (for the pore numbered as 1, 2 and 3) in TGCN model with 10 nanopores. The charges are calculated using the NBO scheme.



**Figure S5.** Representative atomic charges (for the pore numbered as 1 and 2) in HGCN model with 6 nanopores. The charges are calculated using the NBO scheme.