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Supplementary Material

DFT ANALYSIS OF FENETHYLLINE (CAPTAGON): INVESTIGATING ITS INTERACTION WITH GRAPHENE AS A POTENTIAL ADSORBENT

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Table S1. Computational details: A comprehensive summary of all simulation settings and parameters (including those from DFT, Monte Carlo, MD, and GULP optimizations)

DFT calculations (DMol3)	
Parameter	***Value***
Functional	M11L
Basis set	DNP (Double Numerical with Polarization basis set)
Spin treatment	Unrestricted
Total charge	0
SCF density convergence	1×10^{-6} [e/Å³]
Geometry optimization cutoff	1×10^{-5} [Ha]
Global orbital cutoff	3.7 [Å]
Max displacement	0.300 [Å]
Integration grid	Fine (~9000 pts/atom)

Monte Carlo	
Parameter	***Value***
Force field	Dreiding
Electrostatic cutoff	18.5 [Å]
van der Waals cutoff	18.5 [Å]
Simulation type	Simulated annealing
Steps per cycle	100000 (Number of MC steps per heating/cooling cycle)
Heating cycles	30 (Number of temperature cycles in annealing)
Molecular Dynamic	
Parameter	***Value***
Ensemble	NVT (Constant number of particles, volume, and temperature)
Temperature	298 K (System temperature maintained by the Nose thermostat)
Thermostat	Nose (Temperature control method)
Timestep	1 fs (Time increment per MD step)
Simulation duration	2000 ps [Total run time (2,000,000 steps × 1 fs)
Force field	Dreiding (Empirical potential for intramolecular and intermolecular interactions)
Electrostatic & vdW cutoff	18.5 [Å] (Cutoff distance for non-bonded interactions)
Initial velocities	Random (Velocities assigned based on random distribution at start of simulation)
GULP	
Parameter	***Value***
Forcefield	ReaxFF 6.0 (Reactive force field for bond formation/breaking)
Charges	Forcefield assigned (Charges taken from ReaxFF potential)
Energy (function) tolerance	1.0×10^{-5} [eV] (Threshold for energy change per step)
Max. gradient tolerance	1.0×10^{-4} [eV] (Maximum allowed force on atoms)