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

Supplementary Information

An anisotropic dressed pairwise potential model for the adsorption of noble gases on boron nitride sheets

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Table S1: Lennard-Jones parameters.

System	ε (kcal/mol)	σ (Å)
He-He[1]	0.011	2.64
Ne-Ne[1]	0.066	2.77
Ar-Ar[1]	0.239	3.40
Kr-Kr[2]	0.350	3.68
B-B[3]	0.094	3.45
N-N[3]	0.144	3.36

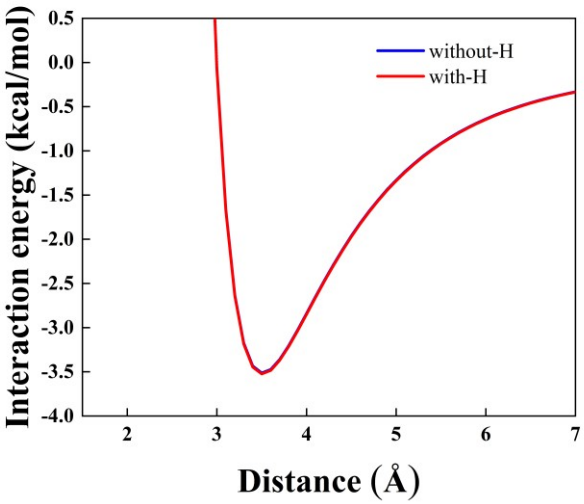

Figure S1: Potential energy profiles evaluated using the LJ potential for the adsorption of Kr on $B_{48}N_{48}H_{24}$, with and without the contributions from the peripheral hydrogen atoms.

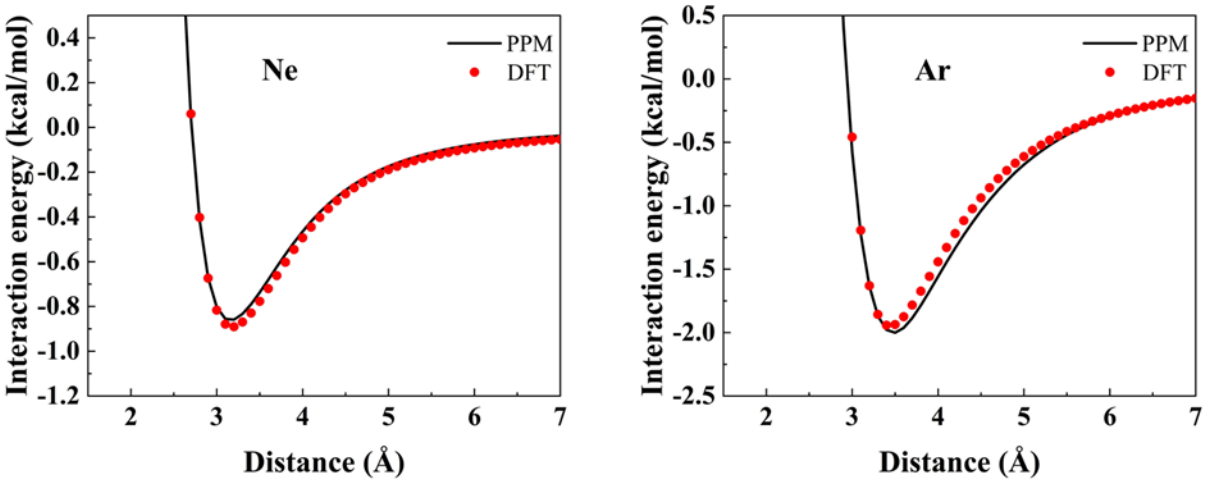

Figure S2: Potential energy profiles for the adsorption of Ne and Ar on top of one of the central B-N bonds of $B_{48}N_{48}H_{24}$ computed using PPM and DFT methodologies.

(b)

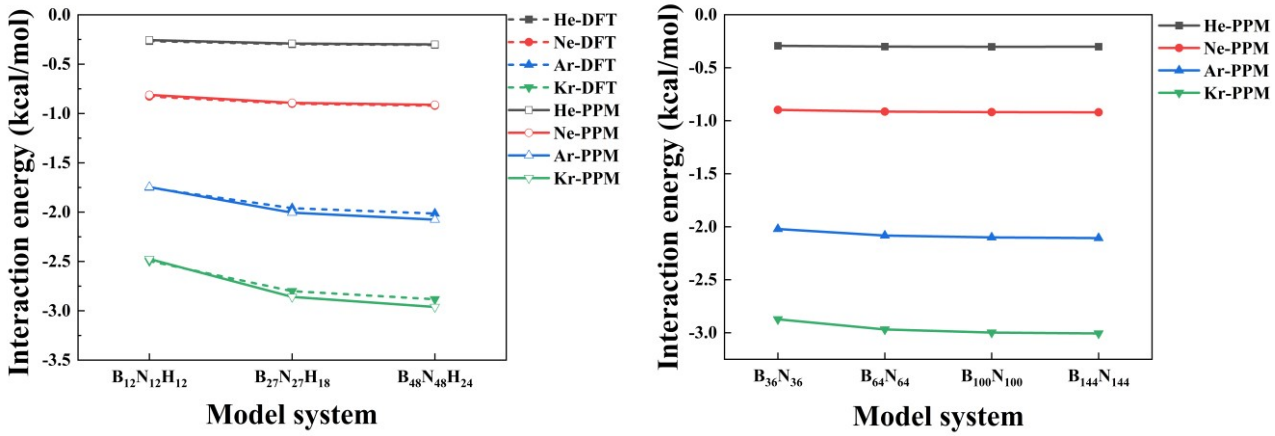

Figure S3: (a) A comparison of the interaction energies evaluated using the DFT and PPM for varying sizes of the molecular models of BN sheets. (b) Convergence of the interaction energies evaluated using PPM with an increase in the size of the BN sheet models obtained using the nanotube generator.[4]

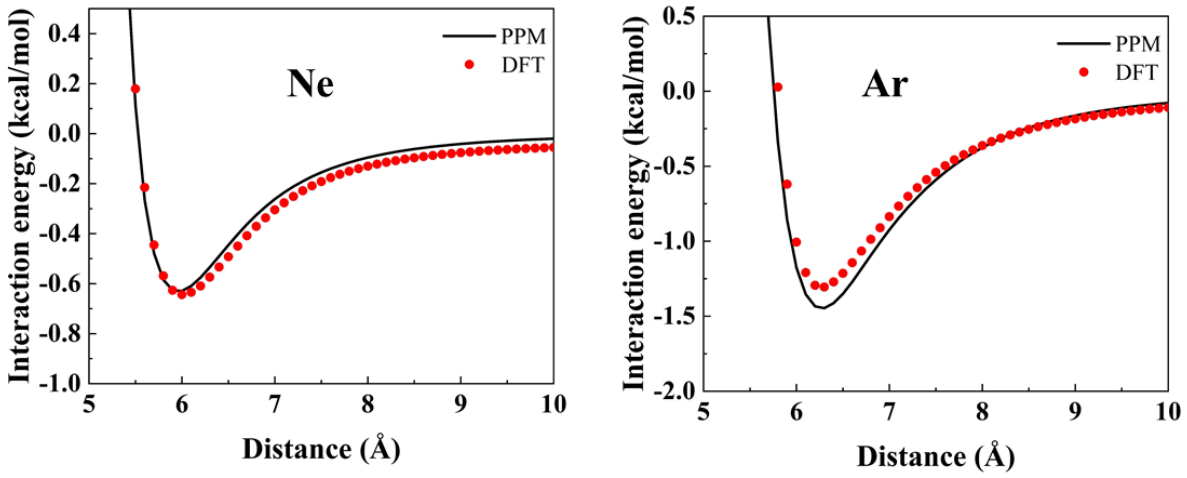

Figure S4: Potential energy profiles for the adsorption of Ne and Ar on the (7,0) BN nanotube computed using PPM and DFT methodologies.

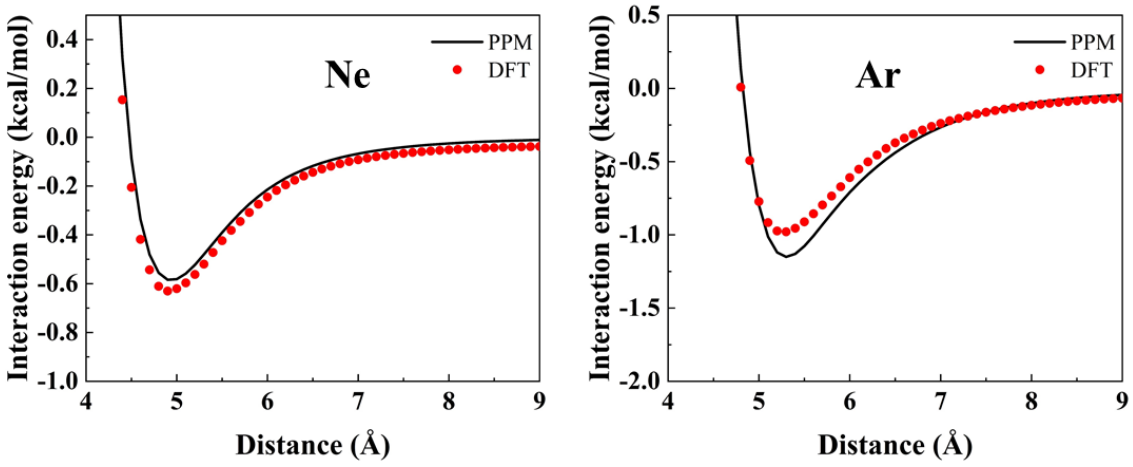

Figure S5: Potential energy profiles for the adsorption of Ne and Ar on the $B_{12}N_{12}$ fullerene computed using PPM and DFT methodologies.

Table S2: Comparison of total interaction energies obtained from DFT optimization with those obtained from single-point energy calculations, both of which are performed on the global minima geometries obtained using the PSO methodology.

System	Single-point energy (kcal/mol)	Energy of optimized geometry (kcal/mol)
Ne_2	-2.079	-2.355
Ne_3	-3.380	-4.241
Ne_4	-4.739	-6.146
Ne_5	-6.069	-8.037

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