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

Computational investigations of stable multiple cage occupancy He clathrate-like hydrostructures

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Supplementary material

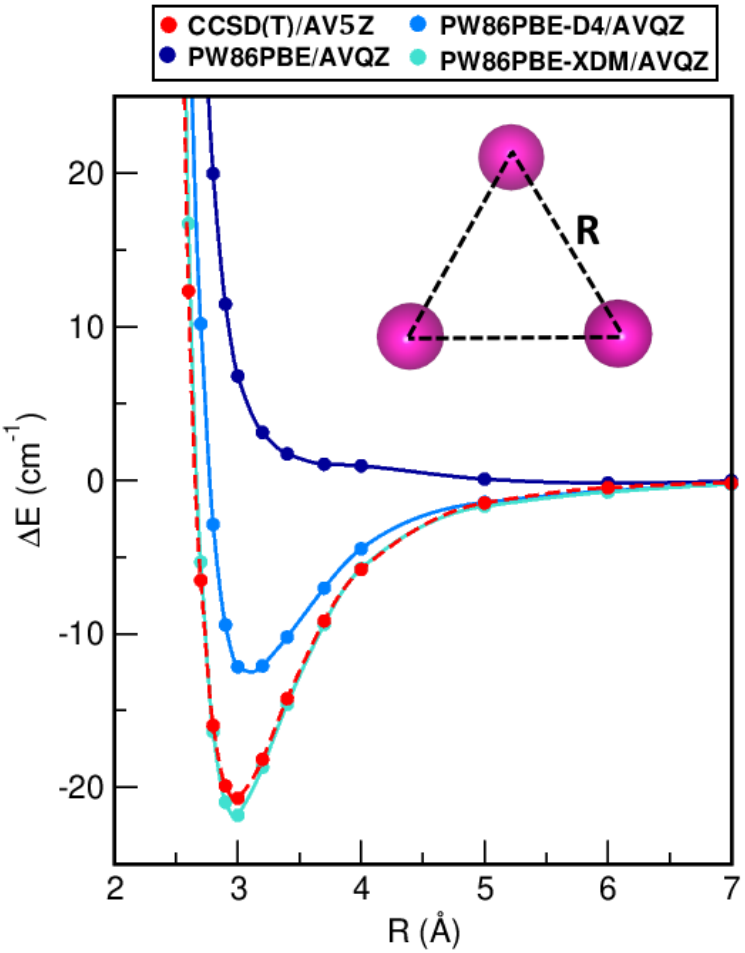

Figure S1: Interaction energies (in cm^{-1}) for the He_3 as a function of He–He distance calculated at the CCSD(T)/AV5Z and PW86PBE(-XDM/D4)/AVQZ levels of theory.

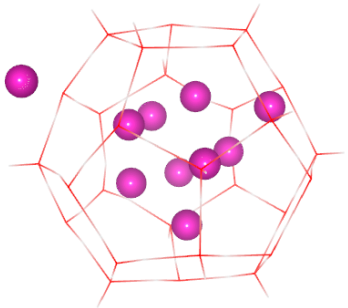

Figure S2: Optimized He_{10}@H structure from PW86PBE/AVTZ calculations.

Table S1: Total energies (in a.u.) of the optimized structures of the isolated He_N atoms from CCSD(T) using the AV6Z, AV5Z, AVQZ and AVTZ basis sets for N=2-4, 5-6, 7-8 and 9, respectively, and PW86PBE/AVQZ calculations.

	E (H)	
N	**CCSD(T)**	**PW86PBE**
1	-2.903	-2.912
2	-5.807	-5.825
3	-8.710	-8.737
4	-11.614	-11.650
5	-14.516	-14.562
6	-17.419	-17.475
7	-20.317	-20.387
8	-23.219	-23.299
9	-26.106	-26.208

Table S2: Total energies (in a.u.) and interaction energies (in cm^{-1}) of the He_N@D systems from PW86PBE/AVTZ optimization calculations.

	PW86PBE				PW86PBE-D4				PW86PBE-XDM			
N	**He_N@D**	**D**	**He_N**	**ΔE (cm^{-1})**	**He_N@D**	**D**	**He_N**	**ΔE (cm^{-1})**	**He_N@D**	**D**	**He_N**	**ΔE (cm^{-1})**
1	-1533.204	-1530.292	-2.912	21.387	-1533.241	-1530.328	-2.912	-174.694	-1533.241	-1530.328	-2.912	-200.426
2	-1536.115	-1530.292	-5.824	265.794	-1536.153	-1530.328	-5.824	-198.169	-1536.153	-1530.328	-5.824	-249.921
3	-1539.024	-1530.292	-8.735	803.349	-1539.063	-1530.328	-8.735	85.555	-1539.063	-1530.328	-8.735	15.826
4	-1541.931	-1530.292	-11.646	1442.066	-1541.972	-1530.328	-11.646	474.275	-1541.973	-1530.328	-11.646	388.727

Table S3: Total energies (in a.u.) and interaction energies (in cm^{-1}) of the He_N@H from optimization PW86PBE/AVTZ calculations.

	PW86PBE				PW86PBE-D4				PW86PBE-XDM			
N	**He_N@H**	**H**	**He_N**	**ΔE (cm^{-1})**	**He_N@H**	**H**	**He_N**	**ΔE (cm^{-1})**	**He_N@H**	**H**	**He_N**	**ΔE (cm^{-1})**
1	-2145.327	-2142.415	-2.912	49.931	-2145.378	-2142.466	-2.912	-131.217	-2145.377	-2142.465	-2.912	-148.278
2	-2148.239	-2142.415	-5.824	27.400	-2148.291	-2142.466	-5.824	-257.015	-2148.290	-2142.465	-5.824	-294.762
3	-2151.150	-2142.415	-8.736	83.572	-2151.203	-2142.466	-8.736	-380.308	-2151.203	-2142.465	-8.736	-442.048
4	-2154.062	-2142.415	-11.648	130.491	-2154.116	-2142.466	-11.648	-514.539	-2154.116	-2142.465	-11.648	-597.346
5	-2156.973	-2142.415	-14.559	315.743	-2157.028	-2142.466	-14.560	-539.019	-2157.028	-2142.465	-14.560	-652.170
6	-2159.884	-2142.415	-17.471	466.469	-2159.940	-2142.466	-17.472	-588.046	-2159.940	-2142.465	-17.472	-722.417
7	-2162.794	-2142.415	-20.383	766.238	-2162.851	-2142.466	-20.383	-515.842	-2162.851	-2142.465	-20.384	-669.403
8	-2165.703	-2142.415	-23.294	1117.406	-2165.762	-2142.466	-23.294	-378.939	-2165.762	-2142.465	-23.295	-554.768
9	-2168.612	-2142.415	-26.205	1731.894	-2168.671	-2142.466	-26.206	-1.653	-2168.672	-2142.465	-26.206	-179.533

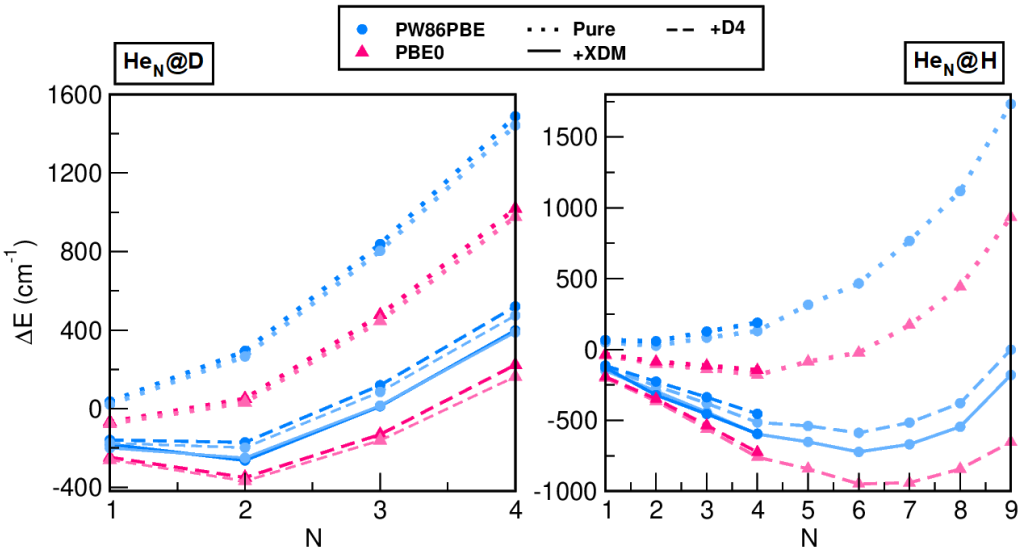

Figure S3: Interaction energies (in cm^{-1}) calculated at PW86PBE and PBE0 levels of theory, with and without dispersion corrections, as a function of the number of the encapsulated He atoms. Dark colors corresponds to AVQZ calculations, while light colors to AVTZ calculations.