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

Assessment of DFT Approaches in Noble Gas Clathrate-like Clusters: Stability and Thermodynamics

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Supplementary material

Table S1: Interaction/cohesive (per water molecule) energies computed at the indicated levels of theory for each He-filled/empty configuration (see Figs. 1 and 2, respectively). Energies are in cm^{-1}.

	Method/Basis set	He@$5^{12}/5^{12}$	He@$4^3 5^6 6^3/4^3 5^6 6^3$	He@$5^{12}6^2/5^{12}6^2$	He@$5^{12}6^4/5^{12}6^4$	He@$5^{12}6^8/5^{12}6^8$
WF-based	**DLPNO-CCSD(T)/AVTZ**	-190.06[a]/-3226.40	-188.60/-3064.42	-140.55/-3158.19	-142.48/-3275.81	-131.57/-3196.33
	DFMP2/CBS[Q5][b]	-169.18[a]/-3115.75	-170.22/-2958.71	-133.59/-3053.03	-125.14/-3173.48	-116.60/-3125.79[c]
DFT-based	**PW86PBE/AVQZ**	36.71/-3000.79	34.10/-2833.09	12.16/-2918.82	67.01/-3045.35	41.24/-2968.75
	PW86PBE-XDM/AVQZ	-181.43/-3340.31	-180.11/-3173.18	-147.54/-3258.41	-127.47/-3380.76	-130.27/-3303.30
	PW86PBE-D4/AVQZ	-158.17/-3341.72	-159.71/-3180.70	-131.22/-3263.93	-112.41/-3386.93	-115.24/-3312.76
	revPBE/AVQZ	51.56/-2129.90	46.80/-1932.60	-18.53/-2039.52	164.26/-2160.98	79.38/-2080.46
	revPBE-D3(0)/AVQZ	-224.28/-2882.43	-227.36/2701.32	-204.88/-2790.89	-161.75/-2911.25	-164.18/-2825.63
	revPBE-D3(BJ)/AVQZ	-251.09/-2836.71	-253.35/-2663.15	-226.45/-2751.63	-149.89/-2867.94	-173.37/-2787.63
	B3LYP/AVQZ	148.87/-2818.78	142.37/-2648.40	95.92/-2747.60	148.55/-3486.72	123.25/-2770.95
	B3LYP-D3(BJ)/AVQZ	-115.02/-3310.85	-118.87/-3152.22	-92.13/-3242.41	-99.58/-3485.00	-87.45/-3478.12
	B3LYP-D4/AVQZ	-82.25/-3267.38	-87.88/-3107.35	-70.91/-3201.63	-71.41/-3322.78	-65.47/-3049.87
	PBE0/AVQZ	-64.86[a]/-3092.53	-67.86/-2939.58	-58.23/-3031.41	-34.19/-3150.02	-45.52/-3077.99
	PBE0-D4/AVQZ	-247.50[a]/-3369.71	-249.03/-3220.33	-195.72/-3311.75	-192.25/-3427.23	-187.23/-3356.92

[a]Interaction energies from ref. 35.
[b]Cohesives energies from ref. 58.
[c]DFMP2/AVQZ / DFMP2/CBS[TQ]

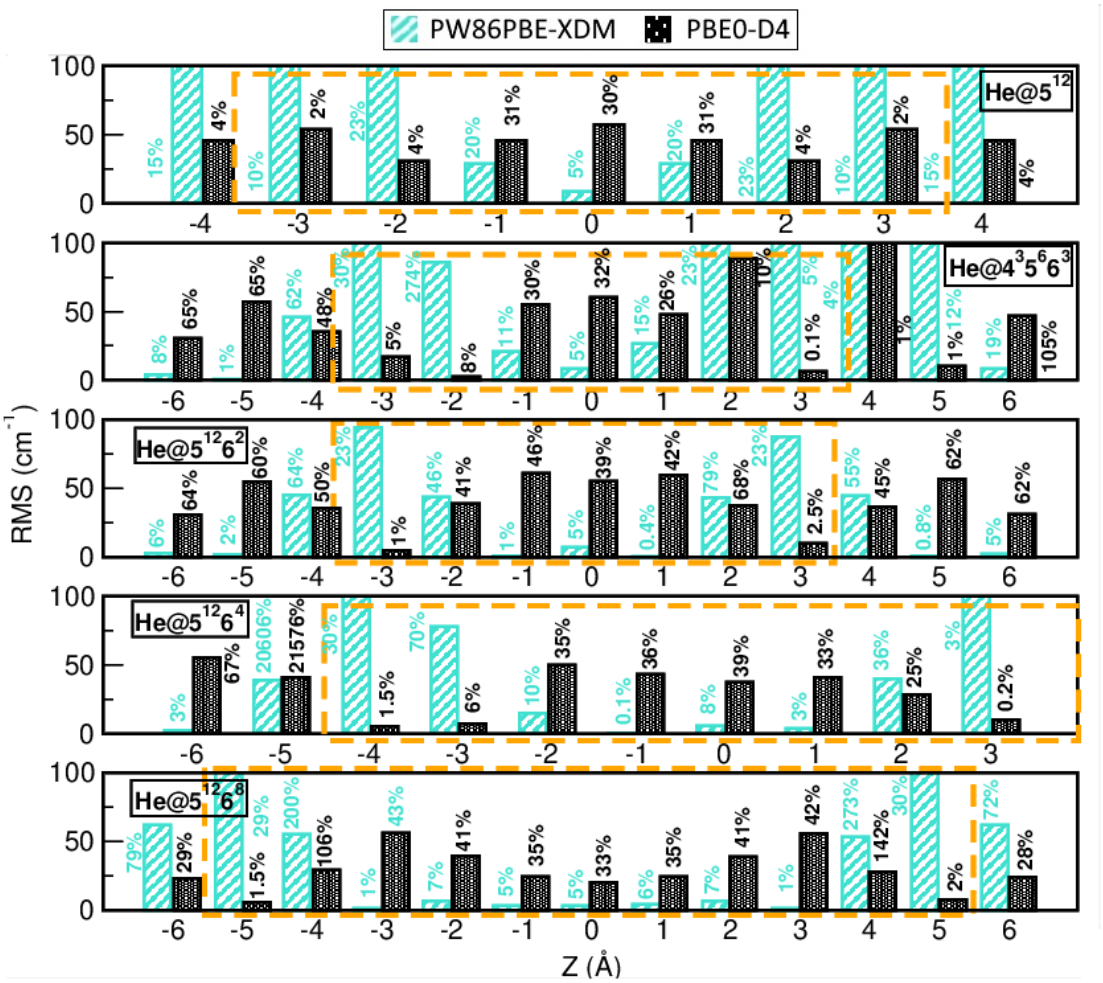

Fig. S1: RMS and % errors of the PBE0-D4 and PW86PBE-XDM energies compared with the DLPNO-CCSD(T)/AVTZ along Z-axis configurations for all He@sI/sII/sH cages studied. Dashed (orange color) boxes indicate configurations inside each cage.