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

Analysing the stability of He-filled hydrates: how many He atoms fit in the sII crystal?

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Supplementary material

Table S1: MEOS fitting results obtained from semi-local (PW86PBE, PW86PBE-XDM, PW86PBE-D4) and non-local functionals (vdW-DF and vdW-DF2) considering empty, single and multiple-cage occupancy of the small and large cages of the sII periodic crystal.

System	Functional	a_0 (Å)	B_0 (GPa)	B'_0	V_0 (Å^3)
sII	**PW86PBE**	17.016	13.98	11.04	4926.50
	PW86PBE-XDM	16.912	15.59	8.35	4837.23
	PW86PBE-D4	16.943	15.29	9.33	4863.68
	vdW-DF	17.480	8.96	4.17	5341.38
	vdW-DF2	17.358	10.84	4.68	5229.71
$He_{(1/1)}$@sII	**PW86PBE**	17.040	13.05	8.87	4947.66
	PW86PBE-XDM	16.903	15.85	8.38	4829.74
	PW86PBE-D4	16.950	15.08	8.86	4869.97
	vdW-DF	17.432	9.15	4.30	5297.35
	vdW-DF2	17.329	10.92	4.81	5203.41
$He_{(1/4)}$@sII	**PW86PBE**	17.064	13.26	9.46	4968.65
	PW86PBE-XDM	16.888	16.14	12.33	4816.75
	PW86PBE-D4	16.960	15.06	10.01	4878.18
	vdW-DF	17.424	9.62	4.44	5289.56
	vdW-DF2	17.315	11.25	4.86	5191.24
$He_{(2/4)}$@sII	**PW86PBE**	17.121	12.61	9.14	5018.19
	PW86PBE-XDM	16.937	15.26	11.66	4858.81
	PW86PBE-D4	17.005	14.47	9.76	4917.44
	vdW-DF	17.481	9.76	4.76	5341.55
	vdW-DF2	17.350	11.45	4.83	5222.26