Supporting Information for *Ab initio* Interatomic Potentials and the Classical Molecular Simulation Prediction of the Thermophysical Properties of Helium

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Table S1. VLE Helium Simulation Data from SAAP[PCJS].*

T (K)	p_{vap} (MPa)	σ (MPa)	ρ_V (mol/dm^3)	σ (mol/dm^3)	ρ_L (mol/dm^3)	σ (mol/dm^3)
6.05	0.0017463	1e-07	0.034898	1e-07	79.9100	0.0017
6.22	0.0024282	1e-07	0.047283	1e-07	79.3450	0.0015
6.40	0.0033679	1e-07	0.063919	1e-06	78.8001	0.0011
6.59	0.0046734	1e-07	0.08634	1e-06	78.0881	0.0015
6.79	0.0064696	1e-07	0.11636	1e-06	77.3874	0.0019
7.01	0.0089477	1e-06	0.15641	2e-06	76.5905	0.0017
7.23	0.012332	1e-06	0.20984	3e-06	75.7360	0.0018
7.48	0.016972	1e-06	0.28117	3e-06	74.8475	0.0017
7.74	0.023317	2e-06	0.37610	4e-06	74.0195	0.0017
8.02	0.031982	3e-06	0.50267	8e-06	72.7383	0.0013
8.32	0.043774	5e-06	0.67092	8e-06	71.6288	0.0019
8.65	0.05997	1.1e-05	0.89839	2e-05	70.2383	0.0009
9.00	0.08159	1.4e-05	1.1954	2.7e-05	68.8642	0.0007
9.11	0.08954	9e-06	1.3047	2.5e-05	68.3189	0.0016
9.23	0.09849	2e-05	1.4288	3e-05	67.8058	0.0027
9.34	0.10804	1.2e-05	1.5580	3.2e-05	67.2487	0.0020
9.46	0.11861	1.7e-05	1.7032	3.5e-05	66.7556	0.0018
9.59	0.13030	2.1e-05	1.8620	3.7e-05	66.1884	0.0023
9.71	0.14284	1.9e-05	2.0341	5.5e-05	65.6711	0.0014
9.84	0.15693	2.3e-05	2.2273	6.8e-05	64.8787	0.0019
9.97	0.17228	2.6e-05	2.4374	6.3e-05	64.4431	0.0030
10.11	0.18918	3.3e-05	2.6722	7.4e-05	63.7044	0.0013
10.25	0.20781	3.6e-05	2.9354	8.7e-05	63.0024	0.0018
10.40	0.22798	3.3e-05	3.2202	0.0001	62.1856	0.0023
10.54	0.25030	4.2e-05	3.5370	0.0001	61.3200	0.0024
10.70	0.27510	7e-05	3.8942	0.0002	60.6772	0.0032
10.85	0.30218	5.3e-05	4.2966	0.0001	59.6979	0.0018
11.02	0.33128	6.3e-05	4.7227	0.0003	58.9218	0.0027
11.18	0.36456	8.5e-05	5.2412	0.0003	57.5760	0.0037
11.36	0.40030	0.00010	5.7989	0.0003	56.6769	0.0030
11.53	0.44163	9.2e-05	6.4932	0.0004	55.6782	0.0039
11.72	0.48477	0.00017	7.2336	0.0005	54.0365	0.0054
11.91	0.53304	9.7e-05	8.1166	0.0006	52.6815	0.0045
12.10	0.58726	0.00018	9.1257	0.0008	51.4121	0.0056
12.51	0.71039	0.00020	11.881	0.0017	46.4257	0.0127

*σ denotes the standard error.

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Table S2. VLE Helium Simulation Data from SAA3P[PCJS].*

T (K)	p_{vap} (MPa)	σ (MPa)	ρ_V (mol/dm^3)	σ (mol/dm^3)	ρ_L (mol/dm^3)	σ (mol/dm^3)
6.05	0.0019625	1e-07	0.039237	1e-07	79.6366	0.0011
6.22	0.0027192	1e-07	0.052979	1e-07	79.1372	0.0011
6.40	0.0037504	1e-07	0.071242	1e-07	78.3204	0.0016
6.59	0.005172	1e-06	0.095652	1e-06	77.7399	0.0015
6.79	0.007127	2e-06	0.12829	2e-06	77.0522	0.0010
7.01	0.009796	1e-06	0.17159	1e-06	76.0808	0.0010
7.23	0.013447	2e-06	0.22928	2e-06	75.3144	0.0013
7.48	0.018403	6e-06	0.30567	6e-06	74.3639	0.0016
7.74	0.025197	5e-06	0.40792	5e-06	73.4443	0.0016
8.02	0.034419	7e-06	0.54317	7e-06	72.3515	0.0009
8.32	0.04693	1.1e-05	0.72245	1.1e-05	71.0816	0.0017
8.65	0.06382	1.2e-05	0.96104	1.2e-05	69.6782	0.0011
9.00	0.08749	2.9e-05	1.2922	2.9e-05	68.3081	0.0017
9.11	0.09625	3.5e-05	1.4153	3.5e-05	67.6813	0.0022
9.23	0.10554	3.2e-05	1.5442	3.2e-05	67.1218	0.0013
9.34	0.11572	3e-05	1.6858	3e-05	66.7515	0.0017
9.46	0.12686	4.9e-05	1.8402	4.9e-05	66.1265	0.0016
9.59	0.13933	5.6e-05	2.0162	5.6e-05	65.5121	0.0019
9.71	0.15272	5e-05	2.2006	5e-05	64.9724	0.0017
9.84	0.16768	3.8e-05	2.4116	3.8e-05	64.3470	0.0024
9.97	0.18386	7.5e-05	2.6406	7.5e-05	63.7197	0.0019
10.11	0.20141	7.7e-05	2.8896	7.7e-05	62.9274	0.0021
10.25	0.2210	0.0001	3.1705	0.0001	62.1669	0.0032
10.40	0.2424	0.0001	3.4847	0.0001	61.3085	0.0044
10.54	0.2660	0.0002	3.8282	0.0002	60.6621	0.0040
10.70	0.2929	0.0002	4.2436	0.0002	59.9363	0.0021
10.85	0.3212	0.0002	4.6698	0.0002	58.5805	0.0036
11.02	0.3521	0.0003	5.1593	0.0003	57.5957	0.0035
11.18	0.3871	0.0002	5.7405	0.0002	56.8148	0.0040
11.36	0.4258	0.0006	6.4001	0.0006	55.4379	0.0052
11.53	0.4679	0.0006	7.1304	0.0006	54.3357	0.0069
11.72	0.5138	0.0009	8.0126	0.0009	52.8018	0.0110
11.91	0.5656	0.0017	9.0657	0.0017	50.9429	0.0069
12.10	0.6239	0.0021	10.485	0.0021	49.4702	0.0098

*σ denotes the standard error.

Table S3. Second Virial Coefficients of Helium (dm^3/mol) Calculated for PCJS, SAAP[PCJS], SAAP[PCJS] + Eq. (7), SAAP and SAAPx and Compared with Reference data.

T (K)	Reference Data (Ref. 42)	PCJS	SAAP[PCJS]	SAAP [PCJS] + Eq. (7)	SAAP	SAAPx
10		-60.080	-60.490		-57.842	-58.300
20	-3.0170	-14.294	-14.451	0.70683	-13.148	-13.439
25	0.97359			2.9040		
30	3.5969	-2.4074	-2.5021	4.7439		
35	5.4366			6.1817		
40	6.7862	2.8618	2.7966	7.3005	-1.6385	-1.8503
45	7.8093			8.1797		
50	8.6047	5.7486	5.7010	8.8796	3.4408	3.2724
60	9.7428	7.5227	7.4867	9.9028	6.2134	6.0726
70	10.497	8.6936	8.6660	10.594	7.9113	7.7895
80	11.017	9.5044	9.4829	11.074	9.0278	8.9201
90	11.383			11.383		
100	11.645	10.510	10.497	11.660	9.7976	9.7009
120	11.968	11.065	11.058	11.962	10.746	10.665
140	12.120	11.383	11.379	12.112	11.263	11.194
160	12.195	11.562	11.561	12.173	11.552	11.492
180	12.221	11.657	11.658	12.181	11.711	11.657
200	12.180	11.698	11.700	12.155	11.790	11.742
220	12.132	11.703	11.706	12.107	11.818	11.774
240	12.069			12.045		
250		11.667	11.671		11.812	11.772
260	11.997			11.974		
280	11.919			11.896	11.763	11.728
300	11.816	11.544	11.549	11.837	11.624	11.595
400		11.211	11.216		11.271	11.251
500		10.865	10.869		10.913	10.898
600		10.539	10.542		10.579	10.567
800		9.9682	9.9699		9.9983	9.9906
1000		9.4921	9.4927		9.5171	9.5108
1500		8.5866	8.5861		8.6067	8.5998
2000		7.9324	7.9326		7.9526	7.9424