Supplementary Information for: Effective coarse-grained solid-fluid potentials and their application to model adsorption of fluids on heterogeneous surfaces

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The effective fluid-surface potentials obtained for the different solid surfaces are presented in the following tables: graphitic carbons, in Table 1; solids with a (111) surface, in Table 2; solids with a (110) surface, in Table 4; solids with a (100) surface, in Table 3; solids with a (111) surface containing a vacancy, in Table 5; and with a (110) surface containing chemical periodicities, in Table 6. The potentials and the distances are presented in reduced units, so that $w^* = w/\varepsilon_{\text{ff}}$, $\langle U^* \rangle = \langle U \rangle / \varepsilon_{\text{ff}}$ and $D^* = D/\sigma_{\text{ff}}$. For the sake of reducing space, the potentials are presented up to a maximum $D^* = 2$ in intervals of $0.03\sigma_{\text{ff}}$.

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Table 1 Effective fluid-surface potentials for the interaction of a methane molecule on the surface of graphene and graphite. w^* corresponds to the free-energy averaged (FEA) potential [*cf.* Equation (41) of parent manuscript] at a temperature $T = 118\,\mathrm{K}$ ($T^* \approx 0.8$) and $\langle U^* \rangle$ is the unweighted-average (UA1) potential [*cf.* Equation (42) of parent manuscript].

	Graphene		Graphite			Graphene		Graphite	
D^*	w^*	$\langle U^* \rangle$	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	w^*	$\langle U^* \rangle$
1.904	-0.813	-0.813	-1.058	-1.058	1.222	-4.447	-4.447	-5.177	-5.177
1.878	-0.859	-0.859	-1.114	-1.114	1.196	-4.787	-4.787	-5.553	-5.553
1.852	-0.909	-0.909	-1.174	-1.174	1.169	-5.151	-5.151	-5.954	-5.954
1.825	-0.962	-0.962	-1.238	-1.238	1.143	-5.537	-5.537	-6.380	-6.380
1.799	-1.020	-1.020	-1.306	-1.306	1.117	-5.943	-5.943	-6.828	-6.828
1.773	-1.081	-1.081	-1.378	-1.378	1.091	-6.362	-6.362	-7.293	-7.293
1.747	-1.147	-1.147	-1.456	-1.456	1.064	-6.787	-6.787	-7.765	-7.765
1.720	-1.218	-1.218	-1.540	-1.540	1.038	-7.202	-7.202	-8.231	-8.231
1.694	-1.294	-1.294	-1.629	-1.629	1.012	-7.585	-7.585	-8.668	-8.667
1.668	-1.377	-1.377	-1.725	-1.725	0.986	-7.901	-7.900	-9.041	-9.041
1.642	-1.465	-1.465	-1.828	-1.828	0.959	-8.097	-8.096	-9.299	-9.298
1.615	-1.561	-1.561	-1.939	-1.939	0.933	-8.094	-8.091	-9.362	-9.359
1.589	-1.664	-1.664	-2.059	-2.059	0.907	-7.774	-7.765	-9.111	-9.103
1.563	-1.776	-1.776	-2.187	-2.187	0.881	-6.961	-6.935	-8.374	-8.348
1.537	-1.897	-1.897	-2.326	-2.326	0.854	-5.407	-5.333	-6.900	-6.827
1.511	-2.028	-2.028	-2.475	-2.475	0.828	-2.750	-2.537	-4.329	-4.117
1.484	-2.170	-2.170	-2.637	-2.637	0.802	1.498	2.103	-0.173	0.431
1.458	-2.324	-2.324	-2.811	-2.811	0.776	7.968	9.576	6.198	7.805
1.432	-2.491	-2.491	-3.000	-3.000	0.749	17.685	21.424	15.809	19.547
1.406	-2.672	-2.672	-3.204	-3.204	0.723	32.176	40.057	30.187	38.065
1.379	-2.868	-2.868	-3.424	-3.424	0.697	54.019	69.515	51.907	67.399
1.353	-3.082	-3.082	-3.663	-3.663	0.671	86.634	115.780	84.391	113.532
1.327	-3.313	-3.313	-3.921	-3.921	0.644	135.686	189.968	133.300	187.577
1.301	-3.564	-3.564	-4.200	-4.200	0.618	209.556	308.336	207.016	305.790
1.274	-3.836	-3.836	-4.502	-4.502	0.592	320.348	502.056	317.642	499.343
1.248	-4.130	-4.130	-4.827	-4.827	0.566	488.688	823.774	485.803	820.881

Table 2 Effective fluid-surface potentials for the interaction of a LJ fluid with the (111) surface of a monolayer and a multilayer fcc solid consisting of LJ particles. w^* corresponds to the FEA potential [*cf.* Equation (41) of parent manuscript] at a temperature $T^* = 1$ and $\langle U^* \rangle$ is the UA1 potential [*cf.* Equation (42) of parent manuscript].

	Monolayer		Multilayer			Monolayer		Multilayer	
D^*	w^*	$\langle U^* \rangle$	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	w^*	$\langle U^* \rangle$
2.005	-0.441	-0.441	-0.602	-0.602	1.225	-2.835	-2.835	-3.398	-3.398
1.975	-0.468	-0.468	-0.636	-0.636	1.195	-3.064	-3.064	-3.659	-3.658
1.945	-0.498	-0.498	-0.673	-0.673	1.165	-3.304	-3.303	-3.932	-3.932
1.915	-0.530	-0.530	-0.713	-0.713	1.135	-3.549	-3.548	-4.215	-4.214
1.885	-0.564	-0.564	-0.756	-0.756	1.105	-3.794	-3.791	-4.498	-4.495
1.855	-0.601	-0.601	-0.802	-0.802	1.075	-4.025	-4.019	-4.772	-4.765
1.825	-0.641	-0.641	-0.851	-0.851	1.045	-4.226	-4.210	-5.018	-5.001
1.795	-0.685	-0.685	-0.905	-0.905	1.015	-4.371	-4.330	-5.212	-5.170
1.765	-0.732	-0.732	-0.962	-0.962	0.985	-4.425	-4.321	-5.318	-5.214
1.735	-0.783	-0.783	-1.024	-1.024	0.955	-4.360	-4.115	-5.310	-5.065
1.705	-0.839	-0.839	-1.091	-1.091	0.925	-4.125	-3.578	-5.135	-4.588
1.675	-0.899	-0.899	-1.164	-1.164	0.895	-3.639	-2.491	-4.715	-3.568
1.645	-0.965	-0.965	-1.242	-1.242	0.865	-2.825	-0.567	-3.972	-1.715
1.615	-1.037	-1.037	-1.328	-1.327	0.835	-1.504	2.724	-2.728	1.499
1.585	-1.115	-1.115	-1.420	-1.420	0.805	0.509	8.149	-0.798	6.841
1.555	-1.200	-1.200	-1.520	-1.520	0.775	3.462	16.992	2.066	15.593
1.525	-1.293	-1.293	-1.629	-1.629	0.745	7.706	31.710	6.213	30.213
1.495	-1.395	-1.395	-1.748	-1.748	0.715	13.754	55.296	12.156	53.692
1.465	-1.506	-1.506	-1.877	-1.877	0.685	22.385	94.910	20.673	93.189
1.435	-1.627	-1.627	-2.017	-2.017	0.655	34.719	159.800	32.884	157.952
1.405	-1.760	-1.760	-2.170	-2.170	0.625	51.910	272.014	49.941	270.029
1.375	-1.904	-1.904	-2.336	-2.336	0.595	76.238	465.206	74.122	463.070
1.345	-2.062	-2.062	-2.516	-2.516	0.565	110.344	802.320	108.068	800.021
1.315	-2.233	-2.233	-2.712	-2.712	0.535	157.443	1423.730	154.993	1421.250
1.285	-2.419	-2.419	-2.924	-2.924	0.505	223.826	2581.980	221.187	2579.310
1.255	-2.620	-2.620	-3.153	-3.153	0.475	313.907	4840.490	311.063	4837.610

Table 3 Effective fluid-surface potentials for the interaction of a LJ fluid with the (100) surface of a monolayer and a multilayer fcc solid consisting of LJ particles. w^* corresponds to the FEA potential [*cf.* Equation (41) of parent manuscript] at a temperature $T^* = 1$ and $\langle U^* \rangle$ is the UA1 potential [*cf.* Equation (42) of parent manuscript].

	Monolayer		Multilayer			Monolayer		Multilayer	
D^*	w^*	$\langle U^* \rangle$	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	w^*	$\langle U^* \rangle$
2.005	-0.382	-0.382	-0.559	-0.559	1.225	-2.455	-2.455	-3.096	-3.095
1.975	-0.405	-0.405	-0.591	-0.591	1.195	-2.653	-2.653	-3.331	-3.331
1.945	-0.431	-0.431	-0.625	-0.625	1.165	-2.861	-2.860	-3.579	-3.579
1.915	-0.459	-0.459	-0.661	-0.661	1.135	-3.074	-3.073	-3.835	-3.834
1.885	-0.488	-0.488	-0.701	-0.701	1.105	-3.285	-3.283	-4.094	-4.091
1.855	-0.521	-0.521	-0.743	-0.743	1.075	-3.487	-3.480	-4.345	-4.339
1.825	-0.555	-0.555	-0.788	-0.788	1.045	-3.662	-3.644	-4.575	-4.557
1.795	-0.593	-0.593	-0.836	-0.836	1.015	-3.796	-3.748	-4.767	-4.719
1.765	-0.634	-0.634	-0.889	-0.889	0.985	-3.868	-3.747	-4.903	-4.781
1.735	-0.678	-0.678	-0.945	-0.945	0.955	-3.857	-3.565	-4.960	-4.668
1.705	-0.727	-0.727	-1.007	-1.007	0.925	-3.753	-3.099	-4.930	-4.276
1.675	-0.779	-0.779	-1.073	-1.073	0.895	-3.528	-2.167	-4.786	-3.424
1.645	-0.836	-0.836	-1.144	-1.144	0.865	-3.181	-0.486	-4.526	-1.830
1.615	-0.898	-0.898	-1.222	-1.222	0.835	-2.703	2.349	-4.143	0.911
1.585	-0.966	-0.966	-1.306	-1.306	0.805	-2.001	7.095	-3.545	5.554
1.555	-1.039	-1.039	-1.397	-1.397	0.775	-1.061	14.852	-2.716	13.200
1.525	-1.120	-1.120	-1.496	-1.496	0.745	0.250	27.551	-1.528	25.778
1.495	-1.208	-1.208	-1.603	-1.603	0.715	2.069	47.751	0.160	45.846
1.465	-1.304	-1.304	-1.720	-1.720	0.685	4.635	82.103	2.582	80.055
1.435	-1.409	-1.409	-1.847	-1.847	0.655	8.114	138.953	5.907	136.749
1.405	-1.524	-1.524	-1.985	-1.985	0.625	12.804	235.520	10.430	233.147
1.375	-1.649	-1.649	-2.136	-2.136	0.595	19.116	399.660	16.562	397.103
1.345	-1.786	-1.785	-2.299	-2.299	0.565	27.596	691.630	24.851	688.876
1.315	-1.934	-1.934	-2.476	-2.476	0.535	38.722	1230.360	35.773	1227.390
1.285	-2.095	-2.095	-2.668	-2.667	0.505	52.972	2231.490	49.810	2228.290
1.255	-2.269	-2.269	-2.874	-2.874	0.475	71.299	4199.890	67.917	4196.450

Table 4 Effective fluid-surface potentials for the interaction of a LJ fluid with the (110) surface of a monolayer and a multilayer fcc solid consisting of LJ particles. w^* corresponds to the FEA potential [*cf.* Equation (41) of parent manuscript] at a temperature $T^* = 1$ and $\langle U^* \rangle$ is the UA1 potential [*cf.* Equation (42) of parent manuscript].

	Monolayer		Multilayer			Monolayer		Multilayer	
D^*	w^*	$\langle U^* \rangle$	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	w^*	$\langle U^* \rangle$
2.005	-0.270	-0.270	-0.482	-0.482	1.135	-2.175	-2.173	-3.165	-3.163
1.975	-0.287	-0.287	-0.509	-0.509	1.105	-2.323	-2.321	-3.378	-3.377
1.945	-0.305	-0.305	-0.538	-0.538	1.075	-2.464	-2.461	-3.590	-3.587
1.915	-0.324	-0.324	-0.568	-0.568	1.045	-2.585	-2.576	-3.788	-3.779
1.885	-0.345	-0.345	-0.601	-0.601	1.015	-2.679	-2.650	-3.967	-3.936
1.855	-0.368	-0.368	-0.636	-0.636	0.985	-2.736	-2.648	-4.117	-4.024
1.825	-0.393	-0.393	-0.674	-0.674	0.955	-2.755	-2.522	-4.239	-3.996
1.795	-0.419	-0.419	-0.715	-0.715	0.925	-2.743	-2.189	-4.339	-3.769
1.765	-0.448	-0.448	-0.758	-0.758	0.895	-2.712	-1.536	-4.432	-3.232
1.735	-0.480	-0.480	-0.805	-0.805	0.865	-2.663	-0.338	-4.518	-2.159
1.705	-0.514	-0.514	-0.856	-0.856	0.835	-2.604	1.673	-4.604	-0.284
1.675	-0.551	-0.551	-0.910	-0.910	0.805	-2.510	5.013	-4.666	2.908
1.645	-0.591	-0.591	-0.969	-0.969	0.775	-2.379	10.498	-4.703	8.233
1.615	-0.635	-0.635	-1.033	-1.033	0.745	-2.183	19.465	-4.685	17.029
1.585	-0.683	-0.683	-1.102	-1.102	0.715	-1.927	33.777	-4.615	31.157
1.555	-0.735	-0.735	-1.177	-1.176	0.685	-1.576	58.051	-4.453	55.236
1.525	-0.792	-0.792	-1.258	-1.257	0.655	-1.114	98.285	-4.174	95.263
1.495	-0.854	-0.854	-1.345	-1.345	0.625	-0.549	166.121	-3.774	162.886
1.465	-0.922	-0.922	-1.441	-1.441	0.595	0.182	284.327	-3.169	280.879
1.435	-0.997	-0.996	-1.544	-1.544	0.565	1.147	489.771	-2.255	486.116
1.405	-1.078	-1.077	-1.657	-1.657	0.535	2.340	869.834	-0.984	865.995
1.375	-1.167	-1.166	-1.779	-1.779	0.505	3.746	1586.620	0.721	1582.650
1.345	-1.263	-1.262	-1.912	-1.911	0.475	5.539	2965.370	3.176	2961.340
1.315	-1.368	-1.367	-2.056	-2.055	0.445	7.730	5746.130	6.623	5742.180
1.285	-1.482	-1.481	-2.211	-2.210	0.415	10.274	11538.600	11.376	11535.000
1.255	-1.606	-1.604	-2.379	-2.378	0.385	13.291	24570.400	18.204	24567.400
1.225	-1.738	-1.736	-2.559	-2.558	0.355	16.695	55973.700	27.994	55972.100
1.195	-1.878	-1.876	-2.751	-2.749	0.325	20.517	136641.000	42.464	136641.000
1.165	-2.025	-2.023	-2.954	-2.952	0.295	24.629	360671.000	64.194	360675.000

Table 5 Effective fluid-surface potentials for the interaction of a LJ fluid with a multilayer fcc solid consisting of LJ particles with a (111) surface with a vacancy. w^* corresponds to the FEA potential [*cf.* Equation (41) of parent manuscript] at a temperature $T^* = 1$ and $\langle U^* \rangle$ is the UA1 potential [*cf.* Equation (42) of parent manuscript].

D^*	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$
2.005	-0.599	-0.599	1.315	-2.701	-2.699	0.625	-1.345	268.148
1.975	-0.634	-0.634	1.285	-2.912	-2.910	0.595	-1.449	459.387
1.945	-0.671	-0.670	1.255	-3.140	-3.137	0.565	-1.527	798.514
1.915	-0.710	-0.710	1.225	-3.384	-3.381	0.535	-1.556	1414.740
1.885	-0.753	-0.753	1.195	-3.643	-3.640	0.505	-1.554	2566.950
1.855	-0.798	-0.798	1.165	-3.916	-3.912	0.475	-1.549	4796.400
1.825	-0.848	-0.848	1.135	-4.197	-4.192	0.445	-1.465	9306.190
1.795	-0.901	-0.901	1.105	-4.480	-4.473	0.415	-1.318	18855.200
1.765	-0.958	-0.958	1.075	-4.753	-4.741	0.385	-1.170	40121.800
1.735	-1.020	-1.020	1.045	-4.998	-4.976	0.355	-0.961	90703.100
1.705	-1.086	-1.086	1.015	-5.190	-5.143	0.325	-0.713	219552.000
1.675	-1.159	-1.158	0.985	-5.300	-5.192	0.295	-0.375	580358.000
1.645	-1.237	-1.237	0.955	-5.290	-5.041	0.265	-0.072	
1.615	-1.322	-1.321	0.925	-5.113	-4.563	0.235	0.258	
1.585	-1.414	-1.413	0.895	-4.705	-3.560	0.205	0.676	
1.555	-1.513	-1.513	0.865	-3.972	-1.717	0.175	0.986	
1.525	-1.622	-1.621	0.835	-2.815	1.465	0.145	1.445	
1.495	-1.740	-1.739	0.805	-1.414	6.780	0.115	1.891	
1.465	-1.868	-1.868	0.775	-0.811	15.556	0.085	2.410	
1.435	-2.008	-2.007	0.745	-0.865	29.895	0.055	3.031	
1.405	-2.160	-2.159	0.715	-0.981	53.488	0.025	4.003	
1.375	-2.326	-2.324	0.685	-1.111	92.471			
1.345	-2.505	-2.504	0.655	-1.227	157.565			

Table 6 Effective fluid-surface potentials for the interaction of a LJ fluid with a multilayer fcc solid consisting of LJ particles with a (110) surface with energetic heterogeneities. w^* corresponds to the FEA potential [*cf.* Equation (41) of parent manuscript] at a temperature $T^* = 1$ and $\langle U^* \rangle$ is the UA1 potential [*cf.* Equation (42) of parent manuscript].

D^*	w	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$	D^*	w^*	$\langle U^* \rangle$
2.005	-0.538	-0.538	1.375	-2.021	-2.020	0.745	-5.497	20.863
1.975	-0.568	-0.568	1.345	-2.174	-2.173	0.715	-5.418	38.385
1.945	-0.601	-0.601	1.315	-2.340	-2.338	0.685	-5.256	67.253
1.915	-0.636	-0.636	1.285	-2.520	-2.517	0.655	-4.975	115.459
1.885	-0.673	-0.673	1.255	-2.714	-2.710	0.625	-4.518	197.858
1.855	-0.713	-0.713	1.225	-2.922	-2.917	0.595	-3.826	340.404
1.825	-0.755	-0.755	1.195	-3.143	-3.138	0.565	-2.820	591.690
1.795	-0.801	-0.801	1.165	-3.376	-3.371	0.535	-1.395	1049.840
1.765	-0.851	-0.851	1.135	-3.618	-3.613	0.505	0.587	1906.670
1.735	-0.905	-0.904	1.105	-3.864	-3.858	0.475	3.316	3562.950
1.705	-0.962	-0.962	1.075	-4.104	-4.097	0.445	7.053	6903.190
1.675	-1.024	-1.024	1.045	-4.330	-4.314	0.415	12.275	14006.500
1.645	-1.092	-1.092	1.015	-4.532	-4.486	0.385	19.488	29822.400
1.615	-1.165	-1.164	0.985	-4.704	-4.573	0.355	29.846	67422.500
1.585	-1.243	-1.243	0.955	-4.851	-4.517	0.325	44.811	163527.000
1.555	-1.329	-1.329	0.925	-4.982	-4.222	0.295	67.252	G 430204.000
1.525	-1.422	-1.421	0.895	-5.108	-3.542	0.265	101.715	
1.495	-1.523	-1.522	0.865	-5.232	-2.246	0.235	154.195	
1.465	-1.632	-1.631	0.835	-5.348	0.034	0.205	223.856	
1.435	-1.751	-1.750	0.805	-5.441	3.897	0.175	305.084	
1.405	-1.881	-1.880	0.775	-5.496	10.322	0.145	389.837	