Supporting Materials

Performance Evaluation on Several Exchange-correlation Functional Approximations in Calculations of Alkali–metals and IB Group Metals Pair Potentials

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Table 1. Inter-atomic potential function in body centered cubic alkali-metal *Li* crystal lattice structure calculated by *WC, RPBE, PW91, PBEsol, PBE, LDA* EC functional, respectively.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.1905	1.104	1.334	0.79	1.045	1.11	0.539
0.1992	0.368	0.593	0.386	0.323	0.397	-0.113
0.2078	-0.203	0.005	-0.186	-0.242	-0.173	-0.616
0.2165	-0.612	-0.44	-0.609	-0.658	-0.6	-1.006
0.2338	-1.234	-1.054	-1.218	-1.263	-1.198	-1.537
0.2598	-1.694	-1.567	-1.689	-1.729	-1.678	-1.926
0.2858	-1.872	-1.753	-1.86	-1.893	-1.842	-2.037
0.3031	-1.886	-1.759	-1.87	-1.902	-1.849	-2.025
0.3118	-1.875	-1.744	-1.859	-1.891	-1.837	-2.003
0.3377	-1.799	-1.669	-1.782	-1.812	-1.757	-1.89
0.3464	-1.768	-1.666	-1.749	-1.776	-1.725	-1.841
0.3724	-1.632	-1.509	-1.606	-1.636	-1.579	-1.68
0.3984	-1.482	-1.369	-1.452	-1.48	-1.423	-1.507
0.4244	-1.304	-1.177	-1.275	-1.311	-1.252	-1.333
0.4503	-1.148	-1.052	-1.123	-1.112	-1.093	-1.162
0.4763	-1.003	-0.891	-0.971	-0.999	-0.941	-1.003
0.5196	-0.753	-0.641	-0.718	-0.754	-0.702	-0.764
0.5629	-0.552	-0.452	-0.522	-0.554	-0.508	-0.564
0.6062	-0.402	-0.325	-0.38	-0.4	-0.361	-0.404
0.6495	-0.271	-0.222	-0.263	-0.274	-0.246	-0.282

Table 1. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.6928	-0.168	-0.167	-0.186	-0.174	-0.162	-0.189
0.7101	-0.145	-0.146	-0.162	-0.149	-0.14	-0.162
0.7361	-0.112	-0.111	-0.125	-0.118	-0.111	-0.128
0.7621	-0.084	-0.08	-0.091	-0.092	-0.088	-0.101
0.7974	-0.073	-0.094	-0.098	-0.071	-0.073	-0.081
0.8227	-0.05	-0.056	-0.062	-0.049	-0.049	-0.053
0.866	-0.023	-0.05	-0.049	-0.018	-0.024	-0.027
0.9093	-0.017	-0.029	-0.033	-0.012	-0.015	-0.016

Table 2. Same as in Table 1 but for the body centered cubic alkali-metal *Na* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.2338	2.107	2.709	2.282	2.055	2.299	1.638
0.2425	1.349	1.889	1.501	1.297	1.515	0.924
0.2511	0.748	1.234	0.881	0.697	0.893	0.362
0.2685	-0.112	0.29	-0.006	-0.16	0.003	-0.429
0.2858	-0.653	-0.312	-0.564	-0.694	-0.555	-0.911
0.3031	-0.988	-0.699	-0.914	-1.023	-0.905	-1.197
0.3204	-1.187	-0.925	-1.113	-1.216	-1.105	-1.355
0.3337	-1.291	-1.065	-1.227	-1.315	-1.217	-1.423
0.3464	-1.322	-1.116	-1.265	-1.341	-1.252	-1.433
0.3637	-1.335	-1.133	-1.271	-1.351	-1.26	-1.427
0.3811	-1.325	-1.153	-1.269	-1.334	-1.255	-1.384
0.3984	-1.275	-1.1	-1.21	-1.285	-1.202	-1.327
0.4157	-1.214	-1.05	-1.152	-1.221	-1.141	-1.25
0.433	-1.146	-0.995	-1.089	-1.15	-1.075	-1.169
0.459	-1.054	-0.923	-1.002	-1.048	-0.982	-1.04
0.485	-0.917	-0.779	-0.861	-0.914	-0.844	-0.912
0.5196	-0.77	-0.654	-0.726	-0.761	-0.702	-0.748
0.5629	-0.595	-0.489	-0.553	-0.584	-0.531	-0.566

Table 2. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.6062	-0.441	-0.351	-0.405	-0.432	-0.387	-0.415
0.6322	-0.34	-0.253	-0.316	-0.337	-0.295	-0.34
0.6495	-0.294	-0.219	-0.276	-0.292	-0.256	-0.296
0.6755	-0.238	-0.183	-0.223	-0.238	-0.2	-0.238
0.6928	-0.211	-0.171	-0.195	-0.212	-0.19	-0.205
0.7361	-0.113	-0.093	-0.121	-0.123	-0.108	-0.137
0.7621	-0.095	-0.09	-0.101	-0.102	-0.095	-0.108
0.8227	-0.027	-0.026	-0.049	-0.035	-0.032	-0.056
0.866	-0.023	-0.026	-0.035	-0.025	-0.025	-0.034
0.9093	-0.012	-0.014	-0.022	-0.012	-0.013	-0.019

Table 3. Same as in Table 1 but for the body centered cubic alkali-metal *K* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***PW91***	***RPBE***	***PBEsol***	***PBE***	***LDA***
0.2598	2.449	3.528	2.9	2.417	2.955	1.825
0.2728	2.043	2.998	2.423	2.016	2.473	1.493
0.2858	1.575	2.424	1.898	1.549	1.942	1.091
0.3118	0.663	1.323	0.895	0.635	0.925	0.282
0.3204	0.394	0.998	0.602	0.366	0.627	0.044
0.3464	-0.269	0.199	-0.116	-0.299	-0.103	-0.541
0.3724	-0.69	-0.327	-0.574	-0.719	-0.569	-0.898
0.3984	-0.926	-0.638	-0.833	-0.952	-0.833	-1.082
0.4244	-1.04	-0.807	-0.961	-1.061	-0.963	-1.151
0.4503	-1.077	-0.881	-1.005	-1.091	-1.008	-1.148
0.4677	-1.072	-0.896	-1.003	-1.081	-1.006	-1.12
0.4763	-1.063	-0.895	-0.995	-1.07	-0.997	-1.101
0.5023	-1.018	-0.87	-0.952	-1.019	-0.953	-1.029
0.5196	-0.976	-0.838	-0.911	-0.974	-0.912	-0.973
0.5629	-0.85	-0.73	-0.787	-0.841	-0.785	-0.819
0.6062	-0.713	-0.605	-0.653	-0.698	-0.648	-0.666

Table 3. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***PW91***	***RPBE***	***PBEsol***	***PBE***	***LDA***
0.6495	-0.578	-0.48	-0.522	-0.561	-0.516	-0.524
0.6928	-0.452	-0.364	-0.403	-0.435	-0.395	-0.401
0.7101	-0.406	-0.323	-0.36	-0.389	-0.352	-0.358
0.7361	-0.341	-0.266	-0.301	-0.326	-0.293	-0.298
0.7621	-0.281	-0.218	-0.249	-0.269	-0.241	-0.247
0.7794	-0.244	-0.185	-0.215	-0.234	-0.209	-0.217
0.7967	-0.211	-0.16	-0.187	-0.203	-0.181	-0.189
0.8227	-0.165	-0.129	-0.15	-0.163	-0.145	-0.153
0.8487	-0.128	-0.106	-0.12	-0.129	-0.116	-0.123
0.866	-0.102	-0.087	-0.101	-0.106	-0.097	-0.106
0.892	-0.077	-0.072	-0.08	-0.082	-0.077	-0.083
0.9093	-0.065	-0.064	-0.069	-0.069	-0.066	-0.071

Table 4. Same as in Table 1 but for the body centered cubic alkali-metal *Rb* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.2858	2.21	3.327	2.714	2.188	2.765	1.696
0.3031	1.523	2.49	1.936	1.507	1.984	1.082
0.3204	0.938	1.772	1.277	0.923	1.319	0.555
0.3464	0.241	0.904	0.493	0.224	0.523	-0.073
0.3724	-0.272	0.249	-0.086	-0.293	-0.065	-0.526
0.3897	-0.525	-0.082	-0.37	-0.547	-0.356	-0.743
0.4157	-0.775	-0.426	-0.657	-0.797	-0.649	-0.943
0.433	-0.876	-0.575	-0.771	-0.896	-0.769	-1.014
0.4503	-0.938	-0.677	-0.847	-0.956	-0.845	-1.049
0.4763	-0.978	-0.763	-0.9	-0.99	-0.899	-1.051
0.485	-0.98	-0.778	-0.905	-0.991	-0.904	-1.043
0.5023	-0.972	-0.792	-0.903	-0.979	-0.901	-1.014
0.5196	-0.951	-0.788	-0.885	-0.954	-0.883	-0.974

Table 4. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.5456	-0.902	-0.759	-0.839	-0.9	-0.837	-0.903
0.5629	-0.862	-0.73	-0.801	-0.857	-0.799	-0.85
0.5889	-0.795	-0.676	-0.735	-0.785	-0.732	-0.767
0.6062	-0.747	-0.635	-0.689	-0.736	-0.685	-0.711
0.6235	-0.699	-0.593	-0.643	-0.685	-0.637	-0.655
0.6495	-0.625	-0.527	-0.571	-0.609	-0.564	-0.575
0.6755	-0.554	-0.463	-0.503	-0.536	-0.495	-0.499
0.6928	-0.505	-0.417	-0.455	-0.487	-0.448	-0.451
0.7361	-0.397	-0.321	-0.355	-0.378	-0.346	-0.345
0.7621	-0.338	-0.269	-0.301	-0.321	-0.291	-0.29
0.7794	-0.297	-0.233	-0.263	-0.282	-0.255	-0.257
0.8227	-0.215	-0.169	-0.193	-0.205	-0.185	-0.187
0.8487	-0.172	-0.138	-0.157	-0.167	-0.151	-0.153
0.8747	-0.131	-0.108	-0.124	-0.13	-0.118	-0.125
0.9093	-0.092	-0.085	-0.095	-0.096	-0.089	-0.094

Table 5. Same as in Table 1 but for the body centered cubic alkali-metal *Cs* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.3031	2.038	3.276	2.643	1.999	2.685	1.479
0.3161	1.291	2.429	1.824	1.266	1.871	0.806
0.3291	0.781	1.82	1.245	0.765	1.298	0.355
0.3464	0.359	1.271	0.741	0.348	0.795	-0.01
0.3637	0.083	0.876	0.394	0.071	0.446	-0.246
0.3897	-0.233	0.407	-0.003	-0.248	0.04	-0.514
0.4157	-0.479	0.033	-0.307	-0.498	-0.276	-0.717
0.433	-0.602	-0.157	-0.462	-0.623	-0.433	-0.815
0.459	-0.744	-0.388	-0.639	-0.767	-0.617	-0.92
0.4763	-0.805	-0.498	-0.72	-0.827	-0.699	-0.956

Table 5. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.5023	-0.858	-0.612	-0.788	-0.877	-0.775	-0.97
0.5196	-0.866	-0.647	-0.804	-0.882	-0.792	-0.959
0.5369	-0.861	-0.666	-0.809	-0.875	-0.794	-0.936
0.5456	-0.856	-0.672	-0.806	-0.868	-0.791	-0.921
0.5629	-0.84	-0.677	-0.791	-0.848	-0.78	-0.885
0.6062	-0.764	-0.636	-0.726	-0.765	-0.711	-0.774
0.6495	-0.668	-0.562	-0.633	-0.661	-0.616	-0.651
0.6928	-0.561	-0.471	-0.528	-0.549	-0.511	-0.529
0.7101	-0.519	-0.434	-0.49	-0.507	-0.47	-0.483
0.7361	-0.461	-0.382	-0.431	-0.446	-0.413	-0.418
0.7621	-0.405	-0.331	-0.369	-0.39	-0.36	-0.358
0.7794	-0.361	-0.291	-0.337	-0.345	-0.316	-0.319
0.8054	-0.307	-0.243	-0.286	-0.292	-0.267	-0.268
0.8314	-0.26	-0.204	-0.236	-0.247	-0.225	-0.223
0.8747	-0.175	-0.129	-0.165	-0.167	-0.149	-0.158
0.9093	-0.126	-0.094	-0.122	-0.123	-0.109	-0.117
0.9353	-0.094	-0.073	-0.09	-0.095	-0.085	-0.092
0.9526	-0.076	-0.062	-0.073	-0.079	-0.072	-0.078

Table 6. Inter-atomic potential function in the IB face-centered cubic metal *Cu* crystal lattice structures calculated by *WC, RPBE, PW91, PBEsol, PBE, LDA* EC functional, respectively.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.1909	5.764	7.326	6.734	5.554	6.678	4.003
0.2121	-1.531	-0.159	-0.72	-1.683	-0.953	-2.793
0.2333	-3.935	-2.759	-3.274	-4.039	-3.528	-4.862
0.2457	-4.362	-3.316	-3.795	-4.444	-4.044	-5.14
0.2616	-4.34	-3.414	-3.849	-4.405	-4.096	-5.006
0.2828	-3.917	-3.157	-3.535	-3.966	-3.766	-4.464
0.3041	-3.333	-2.713	-3.041	-3.373	-3.261	-3.804

Table 6. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.3323	-2.564	-2.096	-2.366	-2.599	-2.58	-2.976
0.3536	-2.066	-1.691	-1.92	-2.099	-2.132	-2.447
0.3889	-1.4	-1.155	-1.325	-1.436	-1.536	-1.753
0.4243	-0.926	-0.782	-0.904	-0.965	-1.11	-1.26
0.4596	-0.599	-0.527	-0.606	-0.637	-0.815	-0.918
0.495	-0.384	-0.365	-0.413	-0.417	-0.617	-0.685
0.5303	-0.25	-0.257	-0.286	-0.272	-0.485	-0.528
0.5657	-0.167	-0.184	-0.201	-0.179	-0.397	-0.423
0.601	-0.113	-0.133	-0.143	-0.118	-0.126	-0.354
0.6364	-0.081	-0.095	-0.099	-0.082	-0.087	-0.309
0.6718	-0.054	-0.067	-0.07	-0.054	-0.058	-0.279
0.7071	-0.036	-0.047	-0.05	-0.034	-0.039	-0.26

Table 7. Same as in Table 6 but for the IB face-centered cubic metal *Ag* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.2333	2.514	4.067	3.427	2.335	3.394	1.193
0.2475	-0.913	0.512	-0.114	-1.047	-0.121	-1.923
0.2616	-2.525	-1.241	-1.836	-2.625	-1.827	-3.317
0.2828	-3.272	-2.195	-2.732	-3.335	-2.71	-3.841
2.899	-3.297	-2.288	-2.803	-3.353	-2.779	-3.813
0.3041	-3.17	-2.286	-2.758	-3.214	-2.731	-3.598
0.3182	-2.912	-2.146	-2.574	-2.949	-2.546	-3.275
0.3323	-2.608	-1.948	-2.333	-2.64	-2.306	-2.919
0.3536	-2.149	-1.632	-1.956	-2.182	-1.934	-2.406
0.3889	-1.505	-1.181	-1.411	-1.545	-1.399	-1.7
0.4243	-1.03	-0.841	-0.996	-1.072	-0.991	-1.178
0.4596	-0.693	-0.593	-0.695	-0.733	-0.692	-0.808
0.495	-0.461	-0.423	-0.485	-0.497	-0.482	-0.551

Table 7. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.5303	-0.309	-0.307	-0.342	-0.336	-0.336	-0.373
0.5657	-0.21	-0.224	-0.243	-0.226	-0.233	-0.249
0.601	-0.143	-0.164	-0.175	-0.152	-0.161	-0.166
0.6364	-0.104	-0.122	-0.126	-0.106	-0.115	-0.11
0.6718	-0.071	-0.088	-0.09	-0.071	-0.078	-0.072

Table 8. Same as in Table 6 but for the IB face-centered cubic metal *Au* crystal lattice structure.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	WC	***RPBE***	***PW91***	***PBEsol***	***PBE***	***LDA***
0.2475	0.821	2.342	1.757	0.597	1.673	-0.431
0.2687	-2.917	-1.551	-2.159	-3.066	-2.175	-3.782
0.2828	-3.679	-2.433	-3.019	-3.791	-3.019	-4.376
0.2889	-3.789	-2.609	-3.181	-3.886	-3.173	-4.422
0.3041	-3.688	-2.644	-3.18	-3.763	-3.16	-4.219
0.3182	-3.359	-2.446	-2.942	-3.42	-2.918	-3.805
0.3394	-2.745	-2.024	-2.448	-2.798	-2.425	-3.102
0.3606	-2.144	-1.598	-1.944	-2.194	-1.924	-2.444
0.3889	-1.473	-1.115	-1.373	-1.525	-1.359	-1.719
0.4243	-0.885	-0.709	-0.872	-0.94	-0.864	-1.079
0.4596	-0.529	-0.468	-0.554	-0.574	-0.549	-0.668
0.495	-0.323	-0.316	-0.36	-0.352	-0.351	-0.41
0.5303	-0.202	-0.219	-0.239	-0.217	-0.226	-0.251
0.5657	-0.132	-0.153	-0.165	-0.137	-0.148	-0.153
0.6364	-0.056	-0.069	-0.077	-0.055	-0.061	-0.057
0.6718	-0.036	-0.045	-0.053	-0.035	-0.039	-0.034
0.7071	-0.023	-0.028	-0.034	-0.022	-0.025	-0.02

Table 9. Inter-atomic potential function in alkali-metal *Li* diatomic systems, calculated by *BLYP, HCTH, PBE, PW91, RPBE, and LDA* EC functional, respectively.

Distance/(*nm*)	Inter-atomic Potential Energy/(eV)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.15	1.186	1.186	1.104	1.110	1.199	1.001
0.17	0.184	0.208	0.087	0.096	0.170	0.003
0.2	-0.773	-0.785	-0.885	-0.882	-0.806	-0.963
0.22	-1.130	-1.162	-1.252	-1.246	-1.181	-1.321
0.24	-1.321	-1.371	-1.451	-1.446	-1.386	-1.515
0.26	-1.398	-1.466	-1.538	-1.534	-1.481	-1.594
0.27	-1.406	-1.477	-1.550	-1.546	-1.496	-1.603
0.29	-1.380	-1.457	-1.528	-1.524	-1.480	-1.575
0.33	-1.230	-1.319	-1.375	-1.371	-1.336	-1.416
0.36	-1.081	-1.167	-1.219	-1.215	-1.185	-1.255
0.4	-0.874	-0.949	-0.997	-0.994	-0.969	-1.029
0.45	-0.644	-0.699	-0.742	-0.743	-0.718	-0.770
0.5	-0.457	-0.496	-0.528	-0.527	-0.508	-0.552
0.55	-0.307	-0.334	-0.352	-0.354	-0.338	-0.372
0.6	-0.194	-0.212	-0.218	-0.221	-0.210	-0.232
0.63	-0.145	-0.161	-0.161	-0.165	-0.155	-0.171
0.66	-0.103	-0.117	-0.112	-0.115	-0.110	-0.119
0.69	-0.072	-0.083	-0.078	-0.082	-0.077	-0.082

Table 10. Same as in Table 9 but for the alkali-metal *Na* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(eV)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.18	0.903	1.027	0.741	0.753	0.931	0.443
0.19	0.414	0.551	0.277	0.290	0.451	0.012
0.22	-0.490	-0.394	-0.615	-0.603	-0.486	-0.803
0.24	-0.818	-0.752	-0.950	-0.937	-0.840	-1.106
0.26	-1.013	-0.981	-1.156	-1.145	-1.064	-1.286
0.27	-1.073	-1.060	-1.223	-1.212	-1.139	-1.338
0.28	-1.115	-1.119	-1.269	-1.259	-1.195	-1.372

Table 10. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(eV)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.29	-1.139	-1.158	-1.297	-1.287	-1.230	-1.389
0.3	-1.149	-1.180	-1.310	-1.300	-1.250	-1.392
0.31	-1.147	-1.188	-1.309	-1.298	-1.255	-1.382
0.32	-1.136	-1.185	-1.299	-1.289	-1.251	-1.364
0.35	-1.061	-1.129	-1.222	-1.213	-1.188	-1.266
0.37	-0.991	-1.066	-1.147	-1.139	-1.120	-1.181
0.38	-0.952	-1.029	-1.105	-1.097	-1.082	-1.134
0.4	-0.873	-0.952	-1.018	-1.012	-1.000	-1.040
0.43	-0.745	-0.823	-0.878	-0.871	-0.867	-0.891
0.46	-0.628	-0.700	-0.746	-0.744	-0.738	-0.754
0.49	-0.521	-0.589	-0.623	-0.618	-0.618	-0.628
0.54	-0.367	-0.421	-0.440	-0.441	-0.438	-0.443
0.59	-0.247	-0.288	-0.293	-0.294	-0.292	-0.294
0.63	-0.169	-0.201	-0.198	-0.200	-0.198	-0.199
0.67	-0.111	-0.134	-0.127	-0.130	-0.128	-0.126
0.72	-0.061	-0.077	-0.068	-0.072	-0.071	-0.067

Table 11. Same as in Table 9 but for the alkali-metal *K* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.25	0.660	0.777	0.371	0.377	0.548	0.223
0.28	-0.115	-0.030	-0.298	-0.291	-0.161	-0.467
0.31	-0.509	-0.465	-0.674	-0.665	-0.570	-0.812
0.33	-0.658	-0.632	-0.824	-0.814	-0.734	-0.937
0.35	-0.752	-0.748	-0.923	-0.913	-0.848	-1.011
0.37	-0.799	-0.815	-0.976	-0.964	-0.915	-1.040
0.38	-0.811	-0.837	-0.989	-0.977	-0.935	-1.043
0.39	-0.817	-0.851	-0.995	-0.984	-0.948	-1.040
0.4	-0.815	-0.857	-0.992	-0.981	-0.951	-1.029

Table 11. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.42	-0.800	-0.853	-0.974	-0.962	-0.941	-0.997
0.44	-0.767	-0.830	-0.936	-0.926	-0.912	-0.948
0.48	-0.676	-0.750	-0.830	-0.817	-0.819	-0.826
0.52	-0.571	-0.644	-0.706	-0.701	-0.702	-0.693
0.57	-0.444	-0.510	-0.552	-0.547	-0.554	-0.534
0.62	-0.324	-0.376	-0.401	-0.401	-0.405	-0.386
0.67	-0.222	-0.260	-0.271	-0.274	-0.273	-0.260
0.7	-0.173	-0.205	-0.207	-0.211	-0.210	-0.198
0.73	-0.129	-0.154	-0.152	-0.158	-0.155	-0.145
0.76	-0.094	-0.115	-0.109	-0.113	-0.112	-0.103
0.79	-0.066	-0.082	-0.075	-0.081	-0.078	-0.070

Table 12. Same as in Table 9 but for the alkali-metal *Rb* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.25	2.109	2.223	1.874	1.862	2.102	1.487
0.28	0.604	0.717	0.417	0.413	0.591	0.139
0.31	-0.087	-0.003	-0.251	-0.255	-0.114	-0.459
0.34	-0.437	-0.386	-0.595	-0.594	-0.489	-0.752
0.37	-0.621	-0.599	-0.777	-0.775	-0.692	-0.897
0.39	-0.687	-0.683	-0.843	-0.840	-0.772	-0.941
0.41	-0.717	-0.731	-0.873	-0.869	-0.816	-0.951
0.43	-0.727	-0.756	-0.883	-0.877	-0.836	-0.942
0.46	-0.704	-0.751	-0.854	-0.850	-0.822	-0.892
0.49	-0.656	-0.719	-0.798	-0.790	-0.780	-0.819
0.52	-0.592	-0.656	-0.724	-0.723	-0.712	-0.732
0.55	-0.527	-0.594	-0.646	-0.641	-0.641	-0.645
0.58	-0.459	-0.526	-0.564	-0.559	-0.566	-0.558
0.62	-0.369	-0.427	-0.454	-0.455	-0.458	-0.444

Table 12. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.65	-0.307	-0.360	-0.377	-0.377	-0.383	-0.366
0.68	-0.248	-0.294	-0.303	-0.305	-0.309	-0.292
0.7	-0.214	-0.255	-0.260	-0.263	-0.265	-0.249
0.73	-0.166	-0.201	-0.199	-0.203	-0.205	-0.190
0.76	-0.126	-0.154	-0.149	-0.154	-0.153	-0.141
0.79	-0.093	-0.116	-0.107	-0.111	-0.112	-0.101
0.82	-0.065	-0.084	-0.075	-0.080	-0.079	-0.069

Table 13. Same as in Table 9 but for the alkali-metal *Cs* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.3	0.944	1.048	0.655	0.645	0.854	0.343
0.33	0.261	0.352	0.051	0.046	0.205	-0.181
0.36	-0.136	-0.075	-0.317	-0.323	-0.192	-0.502
0.39	-0.390	-0.359	-0.565	-0.568	-0.465	-0.710
0.42	-0.546	-0.541	-0.720	-0.723	-0.641	-0.831
0.45	-0.629	-0.647	-0.804	-0.805	-0.745	-0.881
0.46	-0.642	-0.665	-0.816	-0.817	-0.763	-0.884
0.47	-0.649	-0.678	-0.822	-0.824	-0.774	-0.882
0.48	-0.654	-0.689	-0.826	-0.827	-0.783	-0.877
0.5	-0.650	-0.702	-0.817	-0.816	-0.786	-0.854
0.53	-0.618	-0.680	-0.776	-0.771	-0.757	-0.794
0.56	-0.572	-0.635	-0.717	-0.722	-0.705	-0.723
0.59	-0.520	-0.589	-0.652	-0.647	-0.649	-0.648
0.62	-0.461	-0.530	-0.579	-0.575	-0.581	-0.568
0.65	-0.399	-0.461	-0.501	-0.503	-0.506	-0.487
0.68	-0.340	-0.397	-0.426	-0.426	-0.432	-0.410
0.7	-0.304	-0.357	-0.378	-0.378	-0.386	-0.362
0.73	-0.246	-0.291	-0.304	-0.307	-0.312	-0.289

Table 13. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.76	-0.197	-0.235	-0.241	-0.245	-0.248	-0.227
0.79	-0.151	-0.183	-0.181	-0.186	-0.188	-0.171
0.82	-0.116	-0.141	-0.136	-0.142	-0.142	-0.127
0.85	-0.084	-0.105	-0.097	-0.101	-0.102	-0.090

Table 14. Inter-atomic potential function in the IB metal *Cu* diatomic systems, calculated by *BLYP, HCTH, PBE, PW91, RPBE, and LDA* EC functional, respectively.

Distance/(*nm*)	Inter-atomic Potential Energy/(eV)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.17	0.979	1.032	0.632	0.554	1.026	-0.257
0.18	-0.512	-0.393	-0.829	-0.898	-0.478	-1.596
0.19	-1.422	-1.266	-1.714	-1.774	-1.400	-2.374
0.2	-1.954	-1.782	-2.225	-2.278	-1.945	-2.794
0.21	-2.239	-2.065	-2.491	-2.538	-2.241	-2.983
0.22	-2.365	-2.198	-2.601	-2.642	-2.378	-3.026
0.23	-2.388	-2.233	-2.609	-2.645	-2.410	-2.977
0.24	-2.345	-2.206	-2.553	-2.584	-2.376	-2.871
0.25	-2.260	-2.137	-2.456	-2.483	-2.298	-2.732
0.26	-2.151	-2.046	-2.335	-2.359	-2.195	-2.575
0.27	-2.029	-1.941	-2.203	-2.223	-2.077	-2.410
0.28	-1.899	-1.828	-2.063	-2.080	-1.951	-2.243
0.29	-1.768	-1.713	-1.923	-1.937	-1.824	-2.079
0.3	-1.640	-1.600	-1.786	-1.798	-1.698	-1.921
0.32	-1.394	-1.379	-1.522	-1.531	-1.453	-1.623
0.34	-1.174	-1.179	-1.286	-1.291	-1.233	-1.360
0.36	-0.979	-0.999	-1.076	-1.079	-1.035	-1.130
0.38	-0.809	-0.841	-0.892	-0.895	-0.861	-0.931
0.4	-0.665	-0.705	-0.735	-0.736	-0.713	-0.762
0.44	-0.442	-0.489	-0.490	-0.491	-0.481	-0.501

Table 14. contd…

Distance/(*nm*)	Inter-atomic Potential Energy/(eV)					
	BYLP	**HCTH**	**PBE**	**PW91**	**RPBE**	**LDA**
0.48	-0.284	-0.332	-0.315	-0.315	-0.314	-0.317
0.5	-0.225	-0.271	-0.249	-0.249	-0.251	-0.248
0.6	-0.057	-0.077	-0.062	-0.063	-0.067	-0.058
0.7	-0.008	-0.010	-0.009	-0.009	-0.010	-0.008
0.8	0.000	0.000	0.000	0.000	0.000	0.000

Table 15. Same as in Table 14 but for the alkali-metal *Ag* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.2	2.058	2.031	1.663	1.591	2.063	0.757
0.21	0.513	0.573	0.166	0.098	0.528	-0.629
0.22	-0.473	-0.358	-0.781	-0.843	-0.453	-1.477
0.23	-1.088	-0.943	-1.363	-1.420	-1.067	-1.972
0.24	-1.456	-1.297	-1.705	-1.756	-1.438	-2.236
0.25	-1.660	-1.498	-1.887	-1.932	-1.646	-2.350
0.26	-1.755	-1.600	-1.964	-2.005	-1.748	-2.368
0.27	-1.781	-1.638	-1.974	-2.010	-1.781	-2.327
0.28	-1.758	-1.628	-1.937	-1.969	-1.764	-2.244
0.29	-1.705	-1.592	-1.873	-1.901	-1.718	-2.140
0.3	-1.636	-1.539	-1.793	-1.818	-1.655	-2.025
0.32	-1.465	-1.399	-1.604	-1.622	-1.493	-1.778
0.34	-1.284	-1.248	-1.407	-1.421	-1.321	-1.537
0.36	-1.110	-1.098	-1.219	-1.228	-1.152	-1.314
0.38	-0.947	-0.953	-1.042	-1.049	-0.991	-1.110
0.4	-0.800	-0.820	-0.883	-0.890	-0.845	-0.930
0.44	-0.563	-0.602	-0.624	-0.626	-0.606	-0.644
0.48	-0.381	-0.427	-0.423	-0.424	-0.417	-0.427
0.5	-0.309	-0.356	-0.342	-0.342	-0.341	-0.342
0.6	-0.089	-0.118	-0.097	-0.098	-0.104	-0.090
0.7	-0.015	-0.018	-0.015	-0.016	-0.017	-0.013
0.8	0.000	0.000	0.000	0.000	0.000	0.000

Table 16. Same as in Table 14 but for the alkali-metal *Au* diatomic systems.

Distance/(*nm*)	Inter-atomic Potential Energy/(*eV*)					
	BYLP	***HCTH***	***PBE***	***PW91***	***RPBE***	***LDA***
0.19	9.447	8.964	8.829	8.756	9.313	7.601
0.2	5.418	5.143	4.885	4.816	5.329	3.806
0.22	0.996	0.976	0.594	0.531	0.962	-0.237
0.23	-0.138	-0.086	-0.490	-0.548	-0.156	-1.217
0.24	-0.855	-0.757	-1.166	-1.219	-0.863	-1.802
0.25	-1.291	-1.168	-1.569	-1.618	-1.294	-2.125
0.26	-1.544	-1.409	-1.792	-1.837	-1.545	-2.278
0.27	-1.670	-1.533	-1.895	-1.934	-1.671	-2.319
0.28	-1.714	-1.582	-1.918	-1.954	-1.717	-2.288
0.29	-1.705	-1.582	-1.892	-1.924	-1.712	-2.215
0.3	-1.660	-1.549	-1.833	-1.860	-1.670	-2.114
0.32	-1.516	-1.433	-1.663	-1.685	-1.534	-1.875
0.34	-1.338	-1.283	-1.465	-1.481	-1.363	-1.624
0.36	-1.161	-1.131	-1.272	-1.283	-1.192	-1.390
0.38	-0.992	-0.983	-1.088	-1.097	-1.027	-1.175
0.4	-0.837	-0.845	-0.920	-0.929	-0.874	-0.982
0.44	-0.589	-0.618	-0.649	-0.651	-0.625	-0.677
0.48	-0.397	-0.437	-0.438	-0.440	-0.429	-0.447
0.5	-0.323	-0.365	-0.356	-0.357	-0.352	-0.358
0.6	-0.093	-0.121	-0.100	-0.102	-0.107	-0.094
0.7	-0.015	-0.018	-0.015	-0.016	-0.017	-0.013
0.8	0.000	0.000	0.000	0.000	0.000	0.000