

$$U(x; -) = a(x) \frac{- (x)}{-} + b(x) \frac{- (x)^2}{-2} + c(x) \frac{- (x)^3}{-3}$$

x	Omega(x)	a(x)	b(x)	c(x)
	(a. u.)**3	(meV/atom)	(meV/atom)	(meV/atom)
0.00	76.20522757	9738.5763221038	-16230.9605459102	6492.3842102006
0.25	86.80390086	10810.6946305547	-18016.4753008290	7206.4552051858
0.75	106.46856440	14386.5098592601	-23978.7812230421	9591.6389660434
1.00	115.47260489	16349.5885791046	-27249.3142939725	10899.7257148678

$$V_{ij}(R) = \sum_i \frac{O}{P_{ij}^{(1)} @ 1} \frac{R}{R_{ij}^{(1)}} \frac{1_3}{A} \mu^3 R_{ij}^{(1)} i R$$

R_{ij}	P_{CuCu}	P_{AuAu}	P_{CuAu}
(a. u.)	(meV)	(meV)	(meV)
3.60	425.4440207988	0.0000000000	0.0000000000
3.70	4783.5751974674	0.0000000000	0.0000000000
3.80	8087.6739307871	0.0000000000	0.0000000000
3.90	2955.3123119319	0.0000000000	0.0000000000
4.10	-9946.4305930908	0.0000000000	0.0000000000
4.30	-12540.1088650590	0.0000000000	0.0000000000
4.50	-3067.0589270930	0.0000000000	0.0000000000
4.70	-9044.3720626209	0.0000000000	0.0000000000
4.80	-4233.2948548730	-281.4583697546	-51.6078669990
4.90	13245.6961151253	-4411.2550684121	-1897.9083845330
5.00	5125.2628848495	-9662.2406101485	-3657.3601224697
5.10	-2777.3638075472	-10158.4012005519	-2088.1736893219
5.20	-3877.4960541527	-1175.2406190438	-1035.4066509902
5.30	-733.6937701342	7922.8524428707	-328.0526372925
5.40	1231.5084924718	4486.1020143193	2633.2647608399

5. 50	2485.6669178599	-5282.6572572545	2710.7427670617
5. 60	2629.0737924528	10117.2094881190	2021.6367231770
5. 70	2315.6321840812	6125.3992608565	1499.8663346245
5. 80	1807.5426729570	4064.7107813690	1108.5339203663
5. 90	1194.2058567393	4176.9590751528	815.1204042969
6. 00	724.3296961338	3836.4095907721	594.9870940441
6. 10	384.9414504680	2269.1377485809	430.3455872316
6. 20	129.0005418401	948.9694860058	307.9010814410
6. 30	-334.1819209395	68.2312018375	223.4678637986
6. 40	-862.4269454352	-482.3324890671	175.6538848373
6. 50	-1157.8356107900	-805.1931489529	129.5074928203
6. 60	-1277.0797090446	-976.9833230693	86.1126027230
6. 70	-1805.0294538657	-1041.4733246759	55.7690453437
6. 80	-863.1275404942	-938.6068944805	41.0609943372
6. 90	127.5345356750	-672.7587751359	11.5246673998
7. 00	410.5545457114	-500.0846761963	-77.1290259653
7. 10	627.7913945913	-500.2607947487	-446.7912653953
7. 30	989.3303586979	-293.4583793010	-783.7472850040
7. 50	1540.6497409812	136.0909672035	-106.6496635421
7. 70	1506.9013363262	-444.4514075043	458.2280278822
7. 90	450.4156663627	737.1020721682	458.1637252230
8. 10	-810.6910154315	861.3129381781	368.1212128382
8. 30	-905.7598217775	759.5568877965	288.7134519920
8. 50	171.8278679060	821.5767061480	92.2611130164
8. 70	130.4335387480	990.6014633222	-173.9728388553
8. 90	-21.8074793843	932.2651575752	-325.1571619322
9. 10	87.2884129948	777.6923436025	-177.2318823696
9. 30	116.6411134744	307.2296644353	268.0782933718

9. 50	-31.7886184851	-841.1156204316	450.9906874763
9. 70	131.2578542476	51.9810435984	386.4784460956
9. 90	92.0430458675	-55.9562043116	279.5212881330
10. 10	-35.8672857825	-99.4035576517	140.8547737891
10. 30	-157.0662419265	-58.4883004074	42.6743593254
10. 50	-193.7089338831	34.7437442315	-11.0953589200
10. 70	-129.1631515305	161.7400755117	-29.8981649583
10. 90	112.5830470095	7.3719140706	-59.0146156704
11. 10	131.6432006666	153.4021087480	-118.2565278638
11. 30	28.2369735987	299.7817894614	146.0119256456