Supporting information for "Analytic Potential Energy Functions for Simulating Aluminum Nanoparticles," by Ahren W. Jasper, Nathan E. Schultz, and Donald G. Truhlar

November 9, 2004

Parameters for the two best PEFs

See Ref. 16 for a description of the functional forms.

PEF	Parameter	Ref. 16	Present work
NP-A	D_e (eV)	1.710	1.710
	R_e (Å)	2.689	2.689
	a_1 (Å^{-1})	2.345	2.345
	a_2 (Å^{-2})	1.971	1.971
	a_3 (Å^{-3})	0.8773	0.8773
	a	0.1432	0.1432
	R_{CO} (Å)	6.500	6.500
	D'_e (eV)	1.720	1.425
	R'_e (Å)	2.697	4.877
	a'_1 (Å^{-1})	2.243	2.280
	a'_2 (Å^{-2})	2.278	2.601
	a'_3 (Å^{-3})	1.068	1.454
	Δ'	0.1143	0.1382
	R'_{CO} (Å)	6.500	6.500
	κ_1	2.244	4.240
	κ_2	0.1298	0.1177
	κ_3	4.104	4.781
	Δ	1.396	1.640
	γ_1	0.7247	0.7085
	γ_2 (Å)	6.3202	5.396
	d	0.7251	1.133
	γ	0.7373	0.6640
	g_0	6.575	8.545
NP-B	ϕ_0 (eV)	0.3958	0.2095
	R_0 (Å)	2.625	2.760
	E_c (eV)	3.649	2.834
	a	5.194	4.954
	b	4.749	5.203
	c	5.754	5.824
	d	7.664	8.969
	C_0	0.01057	0.4333
	C_1	–7.999	–7.305
	C_2	31.69	29.812
	C_3	–43.63	–54.44
	C_4	28.12	48.41
	C_5	–6.751	–15.50
	s_1	8.658	6.928
	s_2	4.170	3.861
	s_3	27.91	15.50