

Electronic Supplementary Information:

Embedded Atom Model for the Liquid U-10Zr Alloy Based on Density Functional Theory Calculations

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Table S1. Pairwise functions of the EAM potential (eV)

r (Å)	$\varphi_{\text{U-U}}$	$\varphi_{\text{Zr-Zr}}$	$\varphi_{\text{U-Zr}}$
2.0	7.8815	7.6699	
2.2	3.4695	3.8775	2.2561
2.4	1.7588	2.0496	1.4813
2.6	0.9713	1.0782	0.8165
2.8	0.4896	0.5026	0.3542
3.0	0.1682	0.1666	0.0836
3.2	-0.0255	0.0005	-0.0304
3.4	-0.1191	-0.0575	-0.0512
3.6	-0.1409	-0.0762	-0.0509
3.8	-0.1419	-0.0843	-0.0620
4.0	-0.1374	-0.0779	-0.0546

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4.2	-0.1241	-0.0674	-0.0509
4.4	-0.1019	-0.0512	-0.0433
4.6	-0.0737	-0.0385	-0.0367
4.8	-0.0538	-0.0258	-0.0249
5.0	-0.0373	-0.0173	-0.0183
5.2	-0.0232	-0.0120	-0.0155
5.4	-0.0140	-0.0047	-0.0060
5.6	-0.0082	-0.0008	0.0012
5.8	-0.0036	-0.0023	0.0041
6.0	-0.0023	-0.0034	0.0057
6.2	-0.0029	-0.0036	0.0087
6.4	-0.0074	-0.0033	0.0101
6.6	-0.0050	-0.0033	0.0117
6.8	-0.0026	-0.0043	0.0056
7.0	-0.0008	-0.0055	-0.0004

Table S2. Transfer functions of the EAM potential (arbitrary unit)

r (Å)	ρ_U	ρ_{Zr}
2.0	0.234747	0.131352
2.2	0.171140	0.084785
2.4	0.129651	0.060474
2.6	0.089397	0.033720
2.8	0.055878	0.021515
3.0	0.034564	0.017485
3.2	0.023558	0.017978

3.4	0.017806	0.020413
3.6	0.015481	0.016958
3.8	0.012561	0.008864
4.0	0.008589	0.005446
4.2	0.006140	0.004580
4.4	0.006406	0.005951
4.6	0.007599	0.006854
4.8	0.007618	0.007118
5.0	0.007144	0.006983
5.2	0.006641	0.006507
5.4	0.006060	0.007245
5.6	0.005293	0.007068
5.8	0.004717	0.005086
6.0	0.003673	0.003738
6.2	0.002664	0.002704
6.4	0.001258	0.002557
6.6	0.000848	0.002034
6.8	0.000791	0.001081
7.0	0.000891	-0.000151

Table S3. Embedding functions of the EAM potential (eV)

n (a.u.)	F_U	F_{Zr}
0.5	-9.2628	-5.8363
0.6	-10.0276	-6.2740
0.7	-10.5069	-6.5432

0.8	-10.7700	-6.6850
0.9	-10.8924	-6.7851
1.0	-10.9417	-6.8342
1.1	-10.8819	-6.8193
1.2	-10.7293	-6.8790
1.3	-10.5443	-6.9088
1.4	-10.2920	-6.9212
1.5	-9.9569	-6.9045
1.6	-9.4729	-6.8656
1.7		-6.6107

Table S4. Fitted coefficients for the pairwise Morse potential function

	φ_{U-U}	φ_{Zr-Zr}	φ_{U-Zr}
D_0	0.142	0.084	0.078
α	1.081	1.295	1.072
r_e	3.828	3.791	3.956

Table S5. Fitted coefficients for the Chantasiriwan transfer function

	ρ_U	ρ_{Zr}
A	0.732	0.411
B	1.831	1.539
θ	2.340	4.274
β	2.957	3.210

Table S6. Fitted coefficients for the Banerjea embedding function

	F_U	F_{Z_t}
F_0	-10.898	-6.174
γ	0.961	0.753
F_1	-0.060	-0.684