1 SUPPLEMENTARY INFORMATION

1 This appendix includes tabulated data which has been presented and discussed above.

Table A1. The calculated lattice parameter of α-U from 100 K to 800 K.

Temperature (K)	a_0 (Å)	b_0 (Å)	c_0 (Å)	V/at (Å^3)
100	2.72	5.96	4.91	79.75
200	2.74	5.94	4.92	80.22
300	2.78	5.91	4.93	80.83
400	2.80	5.88	4.94	81.27
500	2.82	5.86	4.95	81.67
600	2.82	5.85	4.96	81.95
700	2.83	5.84	4.97	82.33
800	2.84	5.83	4.98	82.63

Table A2. The calculated constant pressure heat capacity of α-U from 100 K to 800 K, compared to experimental values from **?**. Units in J/mol-K.

Temperature (K)	AIMD	Reference
150	27.7	-
250	29.5	26.7
350	30.5	28.7
450	30.7	30.8
550	32.5	33.2
650	34.7	36.2
750	35.1	39.8

Table A3. The interstitial and vacancy formation energy in α-U as a function of temperature. AIMD results are compared to 0 K DFT data (denoted with *) from **?**. Units in eV.

Temperature (K)	Interstitial	Vacancy
0*	4.42	1.69
100	3.81	1.69
200	3.82	1.56
300	3.35	1.32
400	3.13	1.16
500	3.11	1.41
600	3.14	1.23
700	3.30	1.42
800	3.58	1.93

Table A4. The defect-induced strain from interstitials and vacancies as a function of temperature. The strain is defined as $\Delta L/L_0$, where L_0 is the reference length at the given temperature.

	Interstitial			Vacancy		
Temperature (K)	a	b	c	a	b	c
100	0.028	-0.009	0.002	0.000	-0.002	0.000
200	0.020	-0.006	0.002	0.001	-0.002	0.000
300	0.015	-0.004	0.003	-0.003	-0.001	0.000
400	0.008	0.001	0.002	-0.003	0.000	0.000
500	0.008	0.000	0.003	-0.002	-0.001	0.000
600	0.005	0.004	0.002	-0.001	-0.002	0.000
700	0.007	0.000	0.003	0.000	-0.003	0.000
800	0.007	0.000	0.004	0.001	-0.004	0.001

REFERENCES

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