

Calculation of the melting point through free-energy curves was done in ref. 1 (fig. 4) using the same potential file as provided here (as can be seen in ref. 2). The authors quote  $T_m = (276.13 \pm 0.03) \text{ K}$ , which is consistent with the value of  $275 \pm 1 \text{ K}$  in the original paper for the potential [3].

**Table 1:** All densities quoted are in units of  $\text{g} \cdot \text{cm}^{-3}$ . Error bars are standard error of the mean.

Source	$\rho_{\text{liquid}}(274.6 \text{ K})$	$\rho_{\text{liquid}}(298 \text{ K})$	$\rho_{\text{liquid}}(250 \text{ K})$	$\rho_{\text{ice}}(274.6 \text{ K})$
Original paper [3]	1.001	0.997	1.003	0.978
Our calculations	$1.002 \pm 0.001$	$0.998 \pm 0.001$	$1.002 \pm 0.001$	$0.979 \pm 0.001$

## References

- [1] R. P. Leite and M. de Koning, “Nonequilibrium free-energy calculations of fluids using lammmps,” *Computational Materials Science*, vol. 159, pp. 316–326, 2019.
- [2] <https://github.com/plrodolfo/FluidFreeEnergyforLAMMPS>.
- [3] V. Molinero and E. B. Moore, “Water modeled as an intermediate element between carbon and silicon,” *The Journal of Physical Chemistry B*, vol. 113, pp. 4008–4016, 2008.