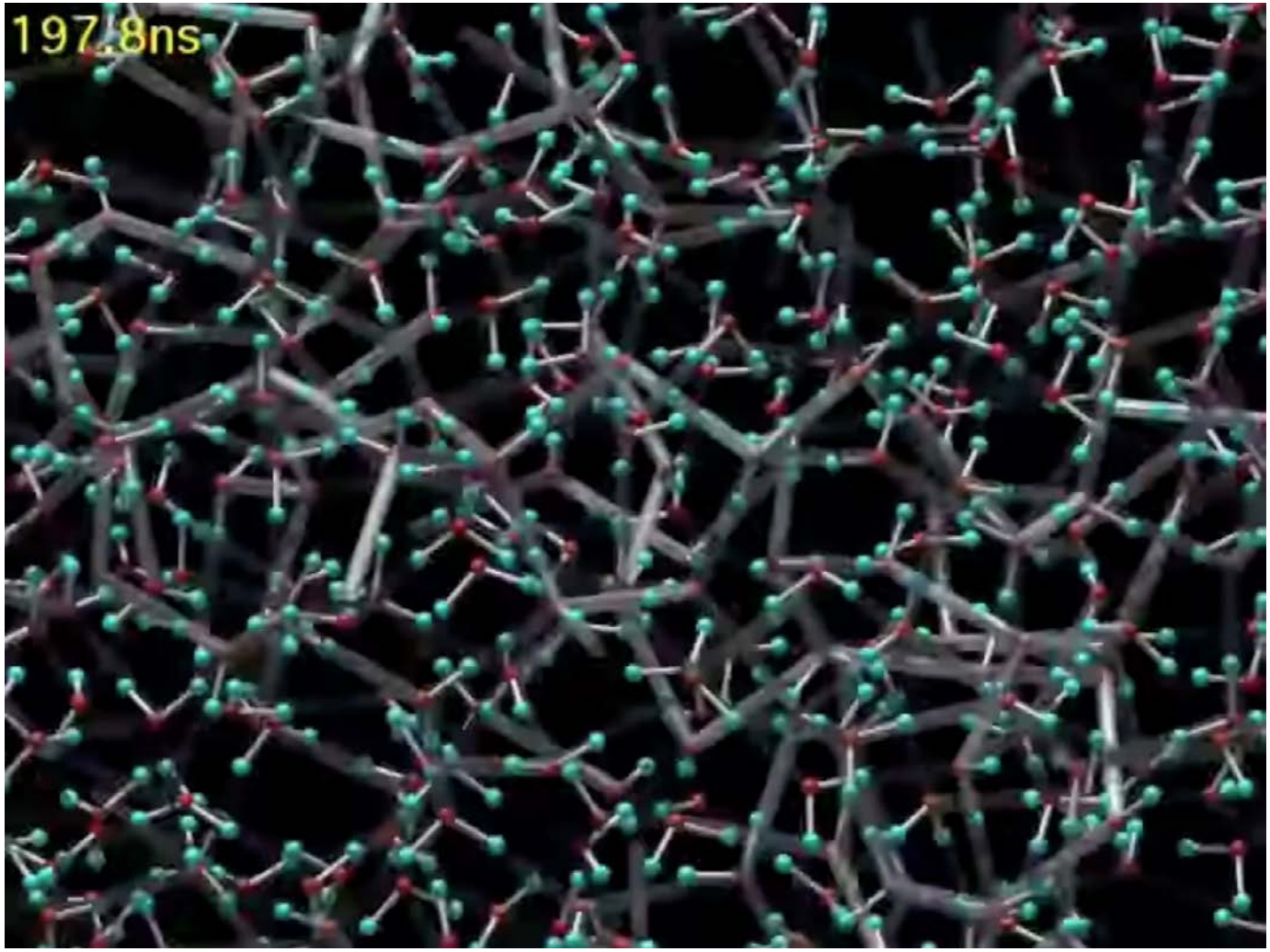
Molecular Dynamics of Water Freezing



https://www.youtube.com/watch?v=gmjLXrMaFTg

M. Matsumoto et al., *Nature* **416**, 409 ('02)

Nucleation Theory

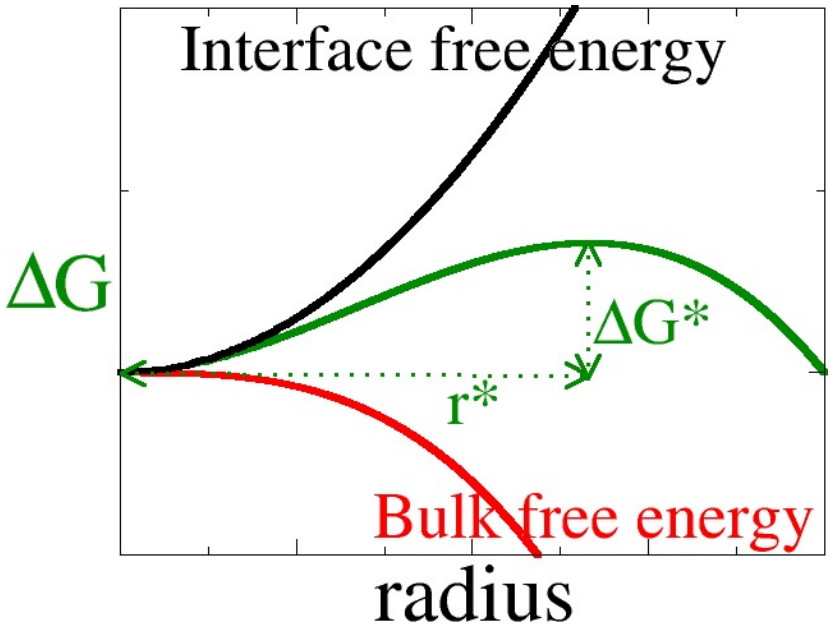
- **Emergent ice cluster in supercooled water has lower free energy (∝ volume) compared to surrounding liquid, but has interfacial energy penalty (∝ surface)**

free-energy difference — $\Delta G = -\frac{4\pi}{3} r^3 |\Delta g| + 4\pi r^2 \sigma$ — surface tension

cluster radius; free-energy-density difference

$$\frac{d\Delta G}{dr} = -4\pi r^2 |\Delta g| + 8\pi r\sigma = 0 \quad \Rightarrow \quad r^* = \frac{2\sigma}{|\Delta g|}$$

- **Nucleation of a cluster above critical radius r^* will grow to the entire system**



https://en.wikipedia.org/wiki/Classical_nucleation_theory