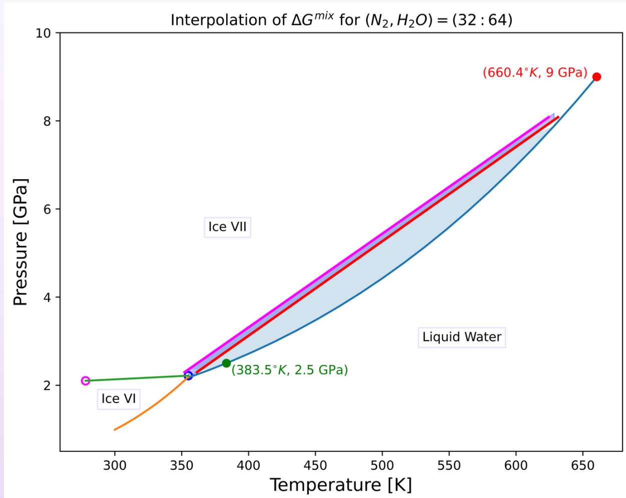
Nitrogen Outgassing in Water Worlds

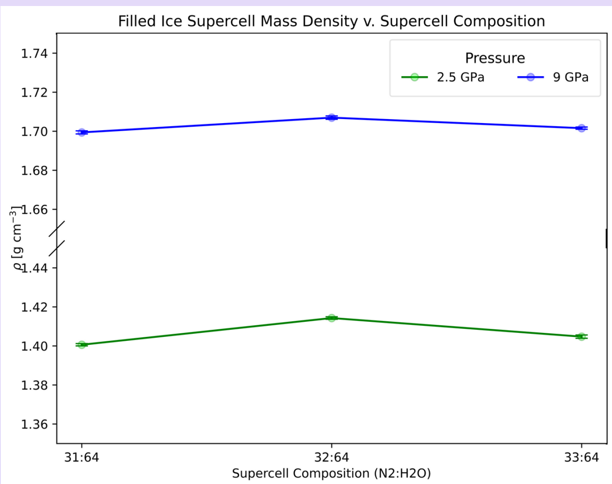
Refath Bari & Amit Levi

BRAUDE College of Engineering, Karmiel

Nitrogen is thermodynamically stable

We find that molecular nitrogen has a negative free energy of mixing with water at 2.5 GPa and 383.5 K, consistent with pressure-temperature domains of small water worlds. To calculate the Gibbs free energy, the enthalpy was calculated via ab-initio DFT-MD simulations. To model the entropy of mixing of water and nitrogen, we adopted the Van Der Waal and Platteuw's standard partition function for nitrogen filled ice, wherein the partition function for the entire structure consists of the canonical partition function for the solvent (hydrogen-bonded water cages) and grand canonical partition function for the guest molecules. This entropy model was thereafter simulated by inputting the volume of filled ice as a function of composition.





Nitrogen is gravitationally stable

We find the density of the filled ice of nitrogen to be less than the density of liquid water at a pressure of 2.5 GPa and temperature of 383.5 K, which implies that if molecular nitrogen does indeed form at the seafloor of water worlds, they will subsequently mix with the liquid ocean, discharge, and evaporate into a secondary atmosphere. Enthalpy calculations indicate that the composition of N2 filled ice with a ratio of 32:64 Nitrogen to Water molecules is most stable. Ammonia is also likely to outgas, as indicated by experimental phase diagrams (Lin 2019, Massani 2022)

Takeaways

Nitrogen Filled Ice is thermodynamically stable at conditions found along the seafloor of a water world

Nitrogen and ammonia can outgas from small water worlds