SeaFreeze: Open Source Code for the Self-consistent Thermodynamic Representation of Water, Ice Polymorphs and Aqueous Systems up to Extreme Pressures and Temperatures

Baptiste Journaux[1, S, C], J. Michael Brown[1], Penny Espinoza[1], Tyler Gordon[1], Erica Clinton[1] and Marshall Styczinski[2]

[1]*Earth and Space Sciences, University of Washington, Seattle, WA, U.S.A.*
[2]*Blue Marble Space Institute of Science, Seattle, WA, U.S.A.*
bjournau@uw.edu

SeaFreeze is an open-source code published in 2020 [1] in Python and MATLAB (https://seafreeze.org/). It provides a modular, easy-to-use, and implement toolbox for describing the thermodynamics of water, ices (Ih, II, III, V, VI and VII), and aqueous solutions (H_2O-NaCl, H_2O-NH_3) in the stable and metastable range up to 10,000 K and 1 Mbar. Based on the local basis function framework [2] for representing the Gibbs energies of all phases, SeaFreeze can reproduce most recent and accurate experimental data in sound speed, densities, heat capcities and phase boundaries. It enables fast and internally self-consistent calculations of all equilibrium thermodynamic parameters, such as entropy, specific volume, heat capacities, sound speeds, and chemical potentials among others. A demonstration of the software and how to implement it will be performed. SeaFreeze has facilitated a wide range of applications of accurate water and ices thermodynamics in physical chemistry, planetary science, and medical sciences, which will be briefly discussed.

References

1. Journaux, B., J.M. Brown, A. Pakhomova, I. Collings, S. Petitgirard, P. Espinoza, J. Ott, F. Cova, G. Garbarino, M. Hanfland (2020) Gibbs energy of ices III, V and VI: Wholistic thermodynamics and elasticity of the water phase diagram to 2300 MPa, *J. Geophys. Res. Planets*, 125, doi: e2019JE006176
2. Brown, J.M., (2018) Local basis function representations of thermodynamic surfaces: Water at high pressure and temperature as an example, *Fluid Phase Equilibria*, 463C, 18-31 doi:10.1016/j.fluid.2018.02.001