A quantitative water model for large-scale simulations at life-relevant conditions

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All-atom simulations of large-size biological systems with explicit water come at a tremendous computational cost. To overcome this problem, coarse-grained models aim to represent the system in a simplified manner but keep the essential properties relevant to its behavior. We consider the coarse-grained model initially introduced by Franzese and Stanley (FS) for water monolayers [1, 2]. The model describes the hydrogen bonds at the molecular level, explicitly accounting for the many-body interactions, but coarse-grains the molecular positions. It is analytically tractable [3] and can be equilibrated by efficient cluster Monte Carlo dynamics [4] for large systems (10^7 molecules) at extremely low temperatures (deep supercooling) in a wide range of pressures (both negative and positive) [5]. Here, we extend it to bulk and reparametrize it to quantitatively agree with the experimental water results for density and thermodynamic response functions around ambient conditions, a prerequisite for its use as a solvent in biological simulations. The region of the quantitative agreement extends up to 50 MPa, covering almost all pressure conditions allowing life on Earth in a temperature range that can be as large as 60 degrees around ambient conditions.

REFERENCES

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FIGURES

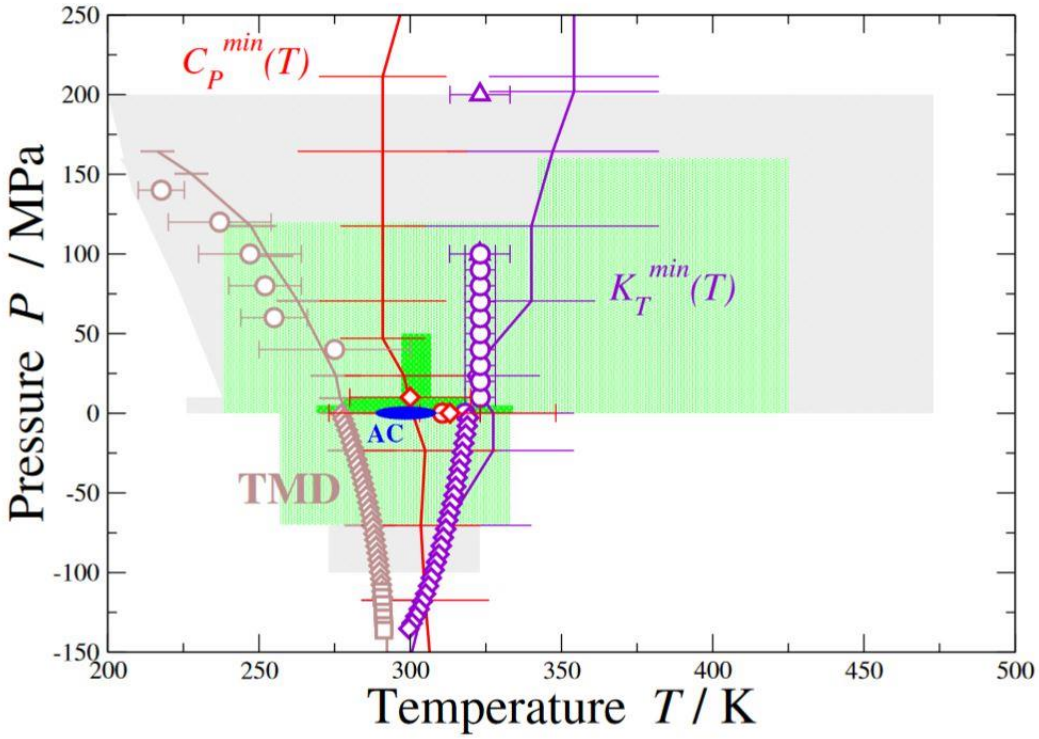

Figure 1: Pressure-Temperature phase diagram of liquid water from experiments (symbols) and the FS model (lines) around ambient conditions (300 K, 1 atm, blue ellipse). The dark-green area marks the thermodynamic region where the model has a complete quantitative agreement with the experimental density, the Temperature of Maximum Density (TMD) along isobars (maroon symbols), the response functions—specific heat (C_P), and isothermal compressibility (K_T)—and their loci of minima (red and violet symbols, respectively). The light-green region is where the model quantitatively agrees with the experimental density but describes the response functions only qualitatively. Experimental data are available only within the grey area.