Efficient Modeling of Thermal and Quantum Fluctuations in Materials and Molecules

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Both electrons and nuclei follow the laws of quantum mechanics, and even though classical approximations and/or empirical models can be quite successful in many cases, a full quantum description is needed to achieve predictive simulations of matter.
Traditionally, simulations that treat both electrons and nuclei as quantum particles have been prohibitively demanding. I will present several recent algorithmic advances that have increased dramatically the range of systems that are amenable to quantum modeling: on one hand, by using accelerated path integral schemes to treat the nuclear degrees of freedom [1], and on the other by using machine-learning potentials to reproduce inexpensively high-end electronic-structure calculations. I will give examples of both approaches, and discuss how the two can be used in synergy to make fully quantum modeling affordable [2].

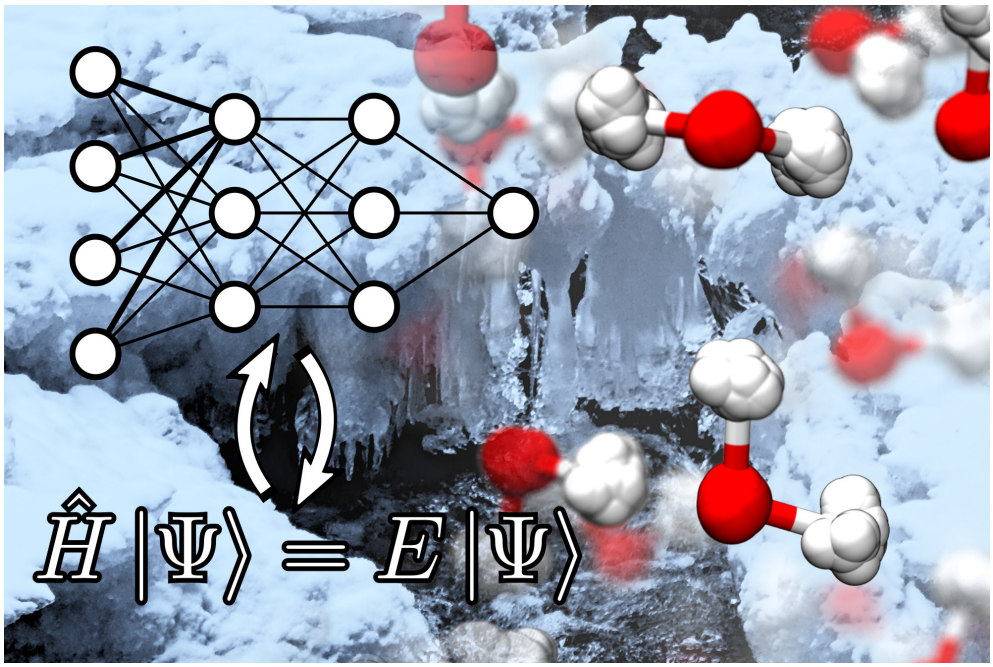

Figure 1: A combination of machine-learning potentials and accelerated simulations of quantum nuclei enable a first-principles description of the thermodynamics of solid and liquid water.

References

1. 1 T.E. Markland and M. Ceriotti, *Nat. Rev. Chem.* **2** (2018), 0109.
2. B. Cheng, E.A. Engel, J. Behler, C. Dellago, and M. Ceriotti, *Proc. Natl. Acad. Sci.* **116** (2019), 1110.