A molecular perspective of water freezing under extreme conditions

Jorge R. Espinosa[1], Chantal Valeriani[2], Alberto Zaragoza[1], Pablo Rosales-Pelaez[1],
Jose Luis F. Abascal[1], Caridad Navarro[1], Carlos Vega[1] and Eduardo Sanz[1]
[1]Dep. Quimica-fisica I, Universidad Complutense de Madrid, 28040 Madrid, Spain
[2]Dep. Fisica Aplicada I, Universidad Complutense de Madrid, 28040 Madrid, Spain

The avoidance of water freezing is the holy grail in the cryopreservation of biological samples, food, and organs. Fast cooling rates are used to beat ice nucleation and avoid cell damage. This strategy can be enhanced by applying high pressures to decrease the nucleation rate, but the physics behind this procedure has not been fully understood yet. We perform computer experiments to investigate ice nucleation at high pressures consisting in embedding ice seeds in supercooled water. We find that the slowing down of the nucleation rate is mainly due to an increase of the ice I-water interfacial free energy with pressure. Our work [1, 2] also clarifies the molecular mechanism of ice nucleation for a wide pressure range. This study is not only relevant to cryopreservation, but also to water amorphization and climate change modeling.

[1] Espinosa, Jorge R., Zaragoza, Alberto, Rosales-Pelaez, Pablo, Navarro, Caridad, Valeriani, Chantal, Vega, Carlos and Sanz, Eduardo, Phys. Rev. Lett. **117**, 135702 (2016).

[2] J. R. Espinosa, C. Navarro, E. Sanz, C. Valeriani, C. Vega, J. Chem. Phys. **145**, 211922 (2016).