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Solvation structure of ice-binding antifreeze proteins HENDRIK HANSEN-GOOS, JOHN WETTLAUFER, Department of Geology and Geophysics, Yale University — Antifreeze proteins (AFPs) can be found in organisms which survive at subzero temperatures. They were first discovered in polar fishes since the 1950's [1] and have been isolated meanwhile also from insects, plants, and bacteria. While AFPs shift the freezing point of water below the bulk melting point and hence can prevent recrystallization; the effect is non-colligative and there is a pronounced hysteresis between freezing and melting. For many AFPs it is generally accepted that they function through an irreversible binding to the ice-water interface which leads to a piecewise convex growth front with a lower nonequilibrium freezing point due to the Kelvin effect.

Recent molecular dynamics simulations of the AFP from *Choristoneura fumiferana* reveal that the solvation structures of water at ice-binding and non-ice-binding faces of the protein are crucial for understanding how the AFP binds to the ice surface and how it is protected from being overgrown [2]. We use density functional theory of classical fluids in order to assess the microscopic solvent structure in the vicinity of protein faces with different surface properties. With our method, binding energies of different protein faces to the water-ice-interface can be computed efficiently in a simplified model.

[1] Y. Yeh and R.E. Feeney, Chem. Rev. **96**, 601 (1996).
[2] D.R. Nutt and J.C. Smith, J. Am. Chem. Soc. **130**, 13066 (2008).

Hendrik Hansen-Goos
Department of Geology and Geophysics, Yale University

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