SEMINARIO DEPARTAMENTO DE QUÍMICA FÍSICA



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Prof. Pablo G. Debenedetti Department of Chemical and Biological Engineering Princeton University

A computational perspective on the metastable phase behavior of liquid water

The preponderance of experimental evidence is consistent with the existence of a metastable first-order transition between two liquid phases in supercooled water [e.g., 1-3].

Computer simulation has played a major role in defining the frontiers of knowledge in this area [4]. Results from a broad range of computational and theoretical approaches, including molecular dynamics [5], free energy calculations [6], the theory of critical phenomena [5], density functional theory [7,8] and machine learning [7,8], support the existence of a metastable critical point in supercooled water. This has important consequences for the observed behavior of ordinary, stable liquid water at ambient conditions.

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