

Entropy in Water

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Abstract: The structure of liquid water is still an open and fascinating question of utmost importance. According to our proposed three-attractor water model, in addition to the familiar two-body interaction based on the linear hydrogen-bond, one should consider two other interactions related to the metastable bifurcated and inverted water dimers. The linear (global minimum) water dimer, and the bifurcated and inverted (local minima) water dimers feature respectively distinct vibrational spectra with quite different different enthalpy and entropy contributions. As a result, in liquid water, unique interplays of enthalpy and entropy could take place, raising the possibility of entropy-driven barriers between attractors.

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