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Understanding liquid water from first principles: a tale of two liquids.[1]

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Despite the simplicity of its molecular structure, condensed phases of water present a complicated phase diagram that has not yet been fully completed. Liquid water as we know it is not a simple liquid. The anomalies of water manifest in many thermodynamic and structural ways. Because of this the complete understanding of the phase diagram of liquid water and ice is still an active area of research in the chemical physics community. In this talk I will present how this problem can be addressed using density functional theory. Our results show that the anomalies of water are strongly linked to the coupling between vibrational and electronic degrees of freedom in the hydrogen bond interaction. And that both electronic and nuclear quantum effects will play a role in the second critical point conjecture.

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