Liquid-liquid phase transition in warm dense hydrogen: a topological approach

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The metallization of solid hydrogen (a molecular insulator) with pressure still remains a challenge for experimental and theoretical physics nowadays [1].

For liquid hydrogen, a insulator-metal transition has been predicted and experimentally measured [2-8]. However, the nature of this transition and its correlation with a first-order liquid-liquid phase transition and the molecular dissociation are still under debate. The study of this transition may have implications for the location of the boundary between a molecular and metallic layer in giant planets and the understanding of their dynamics [9].

In this contribution, the relevant pressure-temperature conditions are thoroughly explored with first-principles molecular dynamics (MD). Both, the generalized gradient approximation of PBE and the van der Waals functional (vdW-DF) are employed for bracketing the true physics in dense hydrogen near dissociation.

Topological analysis of the electron density and the electron localization function (ELF) are performed for snapshots along the MD simulations. These analysis complemented with a percolation theory based on these scalar fields help to a better understanding of the transition.

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