Liquid-liquid transition in high pressure hydrogen by Quantum Monte Carlo methods

C. Pierleoni[a,b]

[a] *Department of Physical and Chemical Sciences, University of L'Aquila, Italy Via Vetoio 10, 67100 L'Aquila, Italy, E–mail: carlo.pierleoni@aquila.infn.it*

[b] *Maison de la Simulation, CEA-Saclay, France, E–mail: carlo.pierleoni@cea.fr*

We studied the transformation from molecular-insulating to monatomic-metallic fluid hydrogen upon increasing pressure, by first principle simulations based on both Density Functional Theory (DFT) and Quantum Monte Carlo (QMC) methods [1,2]. Below a critical temperature $T_c \in [1500\,\mathrm{K}, 3000\,\mathrm{K}]$, the transition is first order with a discontinuity in the specific volume, a sudden dissociation of the molecules and a discontinuous change in electronic properties like the momentum distribution and the electrical conductivity [3,4,5]. Above the critical point the transformation into the metallic dissociated state is continuous. Optical response of the system is obtained within the Kubo-Greenwood framework of DFT. Agreement with recent experimental results at NIF for reflectivity and absorption is observed. Our analysis suggest a coherent picture for apparently discordant experiments from different methods.

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