Improvement of the EoS of Hydrogen and its isotopes based on reflectivity measurements.

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The occurrence of metallization induced by pressure in dense hydrogen was first discussed by Wigner and Hungtington in 1935 [1] for the solid at T=0K. Metallization was also proposed to exist in dense fluid hydrogen [2,3]. The location of the liquid-liquid transition and the magnitude of the volume discontinuity at the transition is still actively debated, both theoretically and experimentally. The nature and location of the transition of dense fluid hydrogen from the molecular state to the plasma state is an essential input in the building of the equation of state of warm dense hydrogen, impacting notably the prediction of the structure of gas giant planets.

Few years ago, we built an equation of state of dense fluid hydrogen using a chemical model to fit ab-initio data provided by Born-Oppenheimer Molecular Dynamic (BOMD) [4]. Even though the improvement over existing EoS tables was significant, the location of the metallization of dense fluid hydrogen remains uncertain. In the fluid phase, the Insulator to Metal Transition (IMT) location strongly depends on the physics that are taken into account in the simulations (long range forces, choice of the xc approximation in BOMD, nuclear quantum effects), leading to an uncertainty of around 300 GPa. Our current project is to use existing experimental data to overcome this uncertainty and so improve the warm dense hydrogen EoS. We will essentially use the data of the shock Hugoniot data in a large range of density-temperature phase space of the IMT, provided by laser-driven shock wave on hydrogen and deuterium precompressed in diamond anvil cells, from 0.1 to 18 GPa [5, 6, 7] and the reverberating bgas gun experiment [8]. We will first show a bentchmark between this new data and our previous BOMD EoS [5], which exhibits some discrepancies, mainly in temperature, at highest precompressions. Reflectivity measurements at 532 nm are also provided in this data, and we show how we infer the ionization rate (Z*) of the material from these measurements, using a mix Drude-Lorentz model for the electrical conductivity. As BOMD simulations always overestimate Z*, we show how we improve our BOMD EoS, using the Z* inferred from the experiments as a new value for the dissociation rate in our chemical model.

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