Equation of state and transport properties of water plasmas from *ab initio* simulations

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The equation of state (EOS) and transport properties of dense water plasmas are of fundamental importance for understanding the interior structure and magnetic-field generation in water-rich giant planets like Uranus and Neptune. *Ab initio* molecular dynamics simulations based on density functional theory (DFT-MD simulations) have proven to be an efficient and accurate method to calculate such thermodynamic and transport properties of water plasmas. This method also allows for a consistent description of transformations from the plasma state to dissociated or molecular fluid states as well as to a superionic solid at high density [1].

This talk will give an overview about the phase diagram, the EOS and the electrical conductivity of warm dense water as derived from DFT-MD simulations. It is shown that the results for the EOS and optical conductivity are in good agreement with shock-wave compression experiments [2].

The description of low-density states ≤ 0.1 g/cm^3 is still hardly feasable with DFT-MD due to computational limitations. Therefore, we also report on investigations on finding a possible region of overlap between DFT-MD data and results from a partially ionized plasma model for low densities [3, 4]. It will be shown that both approaches share a region of reasonable, albeit not perfect overlap, so that the construction of wide-range models for the EOS and conductivity remains yet a challenge.

This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

References

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