

Thermal conductivity of water plasmas from *ab initio* simulations

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The determination of thermal conductivities of dense plasmas is a great challenge for both experimental and theoretical approaches. In partially ionized plasmas, not only electrons contribute to the thermal conductivity but also ions. Here we use *ab initio* molecular dynamics (MD) simulations based on density functional theory (DFT) to calculate the ionic contribution to the thermal conductivity of dense partially ionized water plasmas. The required heat current of the ions is determined by matching the forces from each of the DFT-MD simulations onto effective pair interaction force fields. These force fields are then used to evaluate the Green-Kubo relation for the thermal conductivity using the ion trajectories of the same DFT-MD simulation run. This approach is generally applicable to various multi-component plasmas as well as to materials in liquid, solid, or superionic phases.

For water plasmas the ionic contribution to the thermal conductivity is found to be equal to or greater than the electronic contribution [1] up to temperatures of 20 000 K, depending on the density. The presence of characteristic contributions from thermal dissociation reactions of the water molecules can be traced back to the shapes of the derived force fields between the ionic species. These contributions enhance the ionic thermal conductivity between 3000 and 10 000 K noticeably and are more pronounced toward low densities. Additional benchmark calculations for ice VII and liquid water show good agreement with experimental data and with an *ab initio* study in which the ionic heat current was determined with a generalized variant of density functional perturbation theory for the electronic ground state [2].

Our results are of general significance for understanding thermal transport properties in dense, partially ionized plasmas and other states of matter. The generated thermal conductivity data for water are particularly important for the development of non-adiabatic evolution models for the water-rich giant planets like Uranus and Neptune.

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REFERENCES

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