Contribution ID: **29** Type: **Invited talk**

Electronic transport properties of matter under extreme conditions from density functional theory

Tuesday 22 February 2022 17:30 (30 minutes)

The determination of thermoelectric transport coefficients of dense, partially ionized plasmas is a great challenge for both experiment and theory. In the past two decades, density functional theory (DFT) has evolved to an efficient tool for making theoretical predictions of properties of dense plasmas. Many of these are of high relevance for modelling the interior states, evolution, and magnetic field dynamics of stellar and planetary objects.
Here I will give an overview on the generalized Kubo-Greenwood formalism [1] that is frequently used in calculations of electronic transport properties using the Kohn-Sham states from DFT. Several examples for successful application of this technique to various solid and fluid metals will be presented. Furthermore, a comparison of optical reflectivities of molecular fluids with shock compression experiments [2] will be made. Finally, the limits of the Kubo-Greenwood formalism with respect to its capability of describing electron-electron collisions will be discussed by comparing the thermopower and Lorenz number of weakly degenerate hydrogen plasmas with the known Spitzer results.
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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Session Classification: Session 4