Universität Rostock

Traditio et Innovatio

INSTITUT FÜR PHYSIK

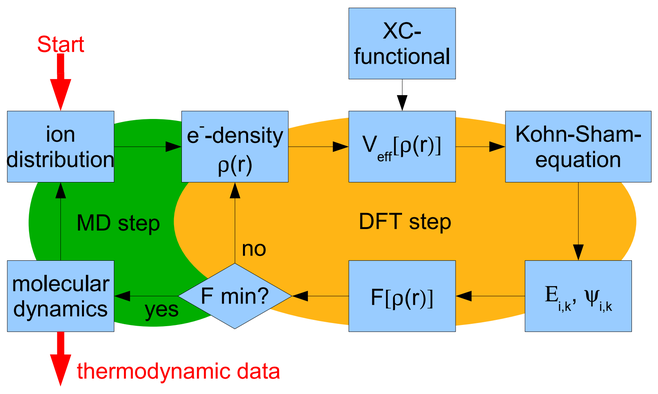
Ab initio simulations for material properties inside Jupiter

Summary

We present new results[1] for thermodynamic material properties as well as for the electrical and thermal conductivity in hydrogen-helium mixtures along the isentrope of Jupiter, for which only relatively simple estimations are available so far. The thermal and electrical conductivities are particularly interesting to examine, since their behavior changes drastically at the transition from the dense nonideal plasma to the molecular fluid. Moreover, these quantities are a fundamental input in magneto-hydrodynamic simulations used to model the magnetic field of Jupiter. Our results cover the range from the outer molecular regions (2000 K, 5 kbar) to the core-mantle boundary (19000 K, 40 Mbar) and are based entirely upon *ab initio* simulations that combine finite-temperature density functional theory (FT-DFT) for the electrons with classical molecular dynamics (MD) for the ions. The underlying planetary isentrope[2] was also derived from *ab initio* equation of state data for hydrogen, helium, and water.

Method

We employ the Vienna *ab initio* simulation package (VASP)[3] which is based upon a quantum treatment of the electrons via FT-DFT (usually with the PBE[4] exchange correlation (XC) functional) to derive forces that act on the ions in a classical MD simulation. At every MD step the ionic motion and the electronic Kohn-Sham wavefunctions $\Psi_{i,\mathbf{k}}(\vec{r})$ and eigenvalues $E_{i,\mathbf{k}}$ are calculated.



Within this approach we can obtain equilibrium properties, such as equation of state data and phase diagrams. Furthermore, transport properties can be derived together with Linear Response Theory.[5] We use the classical Green-Kubo expressions for the ionic transport coefficients. The electronic transport properties are obtained with the expressions derived by Holst *et al.*[6] A key expression is the frequency-dependent Kubo-Greenwood formula to calculate the electronic conductivity,

$$\sigma_e(\omega) = \frac{2\pi e^2}{3m^2\omega V}\sum_{\mathbf{k}} w_{\mathbf{k}} \sum_{j=1}^{N_b}\sum_{i=1}^{N_b}\sum_{\alpha=1}^{3} \left(f_{j,\mathbf{k}} - f_{i,\mathbf{k}}\right) |\langle\Psi_{j,\mathbf{k}}|\hat{p}_\alpha|\Psi_{i,\mathbf{k}}\rangle|^2 \delta(E_{i,\mathbf{k}} - E_{j,\mathbf{k}} - \hbar\omega) \quad .$$

We use both the PBE[4] and the HSE[7] exchange-correlation functionals to calculate the electronic transport coefficients for an ensemble of snapshots taken from simulations with the PBE functional.[4]

Results

Isentrope of Jupiter and thermodynamic material properties

The most abundant element in Jupiter's envelope is hydrogen, mixed with 27.5% (by mass) helium and few heavy elements. Fig. 1 displays the isentrope of Jupiter in the phase diagram of hydrogen. It is located far above the first-order plasma phase transition so that dissociation and ionization happen continuously at temperatures between 4000 to 4500 K.
As the dissociation and ionization occurs, many material properties change drastically (see Fig. 2), e.g., the heat capacities have maxima. This leads to a minimum in the Grüneisen parameter and causes the isentrope to bend in the respective region at 0.9 Jupiter radii, see Ref. 1 for a more detailed description. The discontinuities at 0.63 R_J are due to different element concentrations in the three-layer model[2].

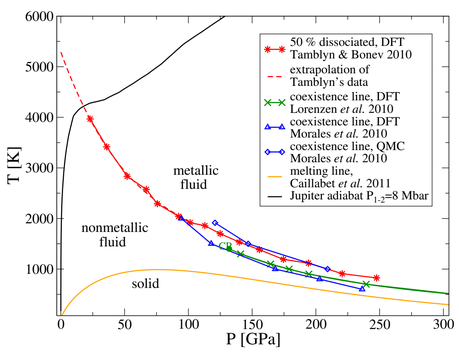


FIGURE 1: Jupiter's isentrope in the phase diagram of hydrogen.

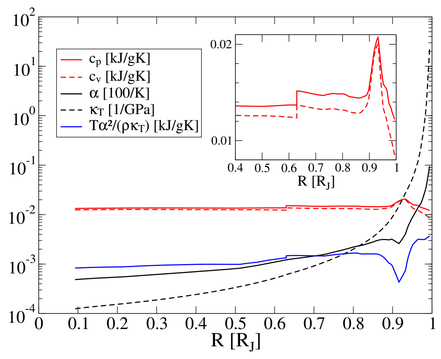


FIGURE 2: Thermodynamic material properties along Jupiter's isentrope.

Electrical (σ) and thermal (λ) conductivity in Jupiter

The exchange-correlation functional can strongly influence the results for the electronic conductivities, because the standard gradient-corrected functionals usually underestimate the fundamental electronic band gap. We therefore use the HSE[7] hybrid functional, that predicts band gaps much more accurately, in the conductivity calculations. The influence of the functional is illustrated in Fig. 3. Strong differences are observed in the molecular region, where the PBE[4] conductivites are one to two orders of magnitude higher than the HSE results.
Furthermore, the influence of the helium concentration is examined in Fig. 4. Both electrical and thermal conductivity decrease when more helium is added. However, the absolute effect is relatively small in the relevant regime around the mean helium concentration.

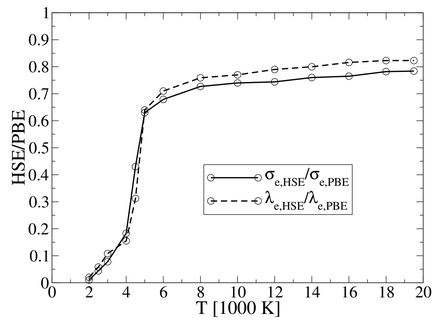


FIGURE 3: Influence of the exchange-correlation functional on electronic transport properties under the interior conditions of Jupiter.

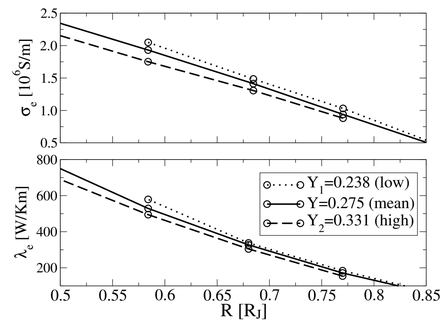


FIGURE 4: Influence of the helium concentration (by mass) on the electronic conductivities near the layer boundary of the Jupiter modele .

The electrical conductivity in Jupiter is displayed in Fig. 5. In the interior of Jupiter, the system is metallic while the transition to the molecular fluid near 0.9 R_J causes the conductivity to drop strongly in the outer regions. Comparison is made with different fully ionized hydrogen plasma models and a semiconductor model fitted to results from gas-gun experiments, see Ref. 1 for references. The electronic thermal conductivity behaves similarly to the electrical conductivity, see Fig. 6. However, the contribution of the nuclei prevents the total thermal conductivity from dropping below 1 W/Km. The thermal diffusivities $\kappa_{e,i} = \lambda_{e,i}/\varrho c_p$ are shown in the lower panel of Fig. 6.

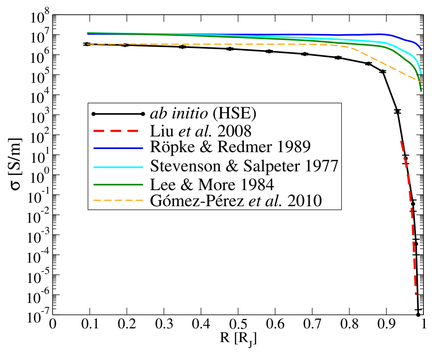


FIGURE 5: Electrical conductivity in Jupiter compared with a selection of other models and estimations.

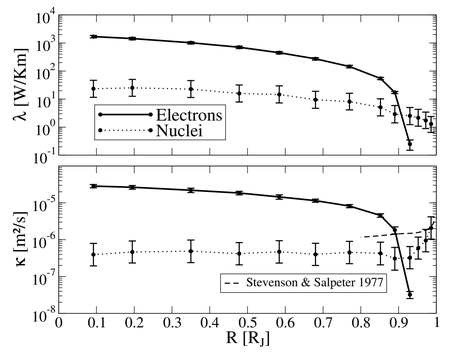


FIGURE 6: *Ab initio* thermal conductivity and diffusivity contributions of electrons and nuclei in Jupiter.

Conclusions and outlook

- For the first time, we have calculated a complete set of thermodynamic and transport properties (electrical and thermal conductivities plus shear and bulk viscosities and diffusion coefficients not shown here) for a planetary model of Jupiter that has likewise been derived with *ab initio* equation of state data for hydrogen, helium, and water.
- Many of the material properties change drastically at the transition from the molecular to the metallic interior, where most of them are relatively constant.
- Our results are of fundamental importance for modelling and understanding the magnetic field of Jupiter[8] and can be used to study other internal processes like core erosion scenarios.
- It will be particularly interesting to apply the whole procedure to Saturn, which is likely to have a more complicated interior structure.[9]

References

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