Iron in Earth's Core and Beyond

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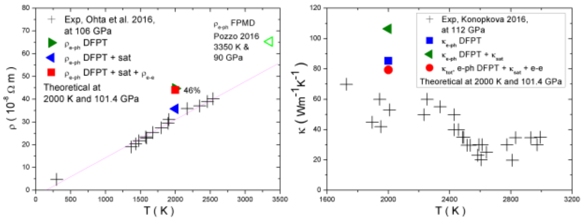
We are performing first-principles studies of transport properties, equations of state, and phase equilibrium in solid and fluid iron and iron-hydrogen mixtures under extreme conditions using density functional theory (DFT) and dynamical mean field theory (DMFT). For transport properties we are using a combination of density-functional perturbation theory (DFPT) with the ABINIT package, first-principles molecular dynamics (FPMD) with QUANTUM ESPRESSO, KKR-CPA, and DMFT. We find that lower pressure (100 GPa) results agree well with experiments, but deviate with increasing pressure and temperatures, suggesting difficulties in extreme condition experiments and with experimental extrapolations. We get good agreement with other theoretical studies when making the same approximations. We will discuss the effects of including saturation effects and higher-order effects that come into play at high temperatures.

We are studying equations of state of Fe-H fluids at extreme conditions to understand giant planetary cores includeing Jupiter and exoplanets. We have performed FPMD for Fe-H systems within DFT up to 30,000 K and 4 TPa. We find complete miscibility in Fe-H fluids at extreme conditions, and non-ideaility is rather small.



Left: Electrical resistivity at 100 GPa. compared with experiment (Ohta et al., 2016). $\rho_{e\text{-}ph}$: electrical resistivity due to electron-phonon scattering calculated by DFPT and Boltzmann transport theory; + sat: including resistivity saturation using the parallel resistor formula; $\rho_{e\text{-}e}$ electrical resistivity due to electron-electron scattering. Right: Thermal conductivity at 100 GPa computed at 2000 K and 100 GPa compared with experimental data at 112 GPa (Konopkova et al., 2016).