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Conductivity and Correlations in Fe at Earth Core Conditions
R.E. COHEN, Carnegie Inst for Science and LMU, PENG ZHANG, Department of Physics, Xi'An Jiaotong University, KRISTJAN HAULE, Dept. Physics, Rutgers University — We have computed electrical conductivity in iron at Earth core conditions self-consistently within many-body theory using DFT/DMFT. We find that electron correlations are important even in the generation of Earths magnetic field. Earth's magnetic field was believed to arise from thermal convection of molten iron alloy in Earth's outer core, but density functional theory (DFT) calculations suggested that the conductivity of iron is too high to support thermal convection, so that new geodynamo models were being developed. The DFT computations for resistivity were based on the scattering of electrons off of atomic vibrations, or electron-phonon (e-p) scattering. We applied self-consistent density functional theory plus dynamical mean-field theory (DFT+DMFT) to iron and found that at high temperatures electron-electron (e-e) scattering is comparable to the e-p scattering, bringing theory into agreement with experiments and solving the transport problem in Earth's core, consistent with the conventional thermal geodynamo [Peng, Cohen, and Haule, Nature 517, 605, 2015]. How electron correlations change with pressure, and how this affects material properties, will be discussed. This work is supported by the US National Science Foundation and the ERC Advanced grant ToMCaT.

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