Thermodynamic, transport, and optical properties of iron in the vicinity of melting from *ab initio* calculations and experiment

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Iron is a widespread component in various types of structural materials, which are exposed to intensive thermal and mechanical loads. So, it is of great importance to obtain reliable data both on equation of state of iron and its transport and optical properties. Nevertheless, thermal expansion and electrical resistivity of iron, especially in liquid state, are still a matter of debate.

In this work, the properties of iron near the melting are found independently from quantum molecular dynamics calculations and from experiments on pulse heating. We pay special attention to the need to take into account the spin polarization in the part devoted to *ab initio* calculations. The thermal expansion curve of iron and the temperature dependence of enthalpy are reconstructed both with and without taking into account spin polarization. The comparison with experiments is presented, including data on enthalpy obtained in our team. Also electrical resistivity and normal spectral emissivity of solid and liquid iron are restored from first-principles calculations using the Kubo–Greenwood formula and the Kramers–Kronig transform.

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