Influence of taking spin polarization into account on ab initio calculations of thermodynamic properties of solid and liquid iron

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The equation of state of iron that is one of important nuclear power plants is essential for analyzing the safety of reactors currently in operation or planned for operation in the future. Generally experimental data of thermal expansion in iron is limited up to the temperature of 2.5 kK with no enough experimental data at higher temperatures. If thermodynamic parameters are such that it is difficult or impossible to conduct an experiment or its results are hardly reproducible, ab initio calculations are used to obtain reliable data on properties of materials. As ab initio quantum molecular dynamic method (QMD), based on density functional theory [1], allows both properties of electronic subsystem and movement of ions, one can use it for modeling of liquid metals behavior. In this work, the analysis of the convergence of the calculation results in terms of simulation parameters is carried out, the curve of thermal expansion of iron in the vicinity of melting in the solid and liquid phases and the curve of the enthalpy versus temperature are reconstructed. Following [2], we analyzed the influence of spin polarization on the thermal properties of iron using the QMD method. This work has been supported by the Russian Science Foundation (grant No. 20-79-10398).

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[2] Korell J A, French M, Steinle-Neumann G and Redmer R 2019 *Phys. Rev. Lett.* **122** 086601