First-principles-based calculations of thermophysical properties of pure elements

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In this work we report on the modelling of thermophysical properties in pure elements using first-principles calculations. Our theoretical approach considers the different physical contributions to the thermophysical properties from electronic excitations, phonons, magnetic excitations, etc. The main contribution is originated from the lattice vibrations or phonons, which can be evaluated using Density Functional Theory (DFT) and the Density Functional Perturbation Theory (DFPT) [1], as implemented for example in the Quantum Espresso code [2]. Using these methods, phonon dispersions can be calculated and compared with experimental results from neutron scattering. Thermophysical properties are then evaluated by thermodynamic integration using both the harmonic and quasi-harmonic approximations [3]. Electronic excitations are then included from DFT-calculated electronic density of states (eDOS) using the Fermi-Dirac statistics. When necessary, the contribution of magnetic excitations can also be included, as well as the contribution from vacancies and anharmonic excitations.

We extensively compare the results of calculations with experiments. Several elements were considered in this work, including Fe, Cr, Al, Ni, Ti, Cu, Co, Re.

[1] S. Baroni, S. de Gironcoli, and A. Dal Corso. Reviews of Modern Physics, 73:515 (2001)

[2] www.quantum-espresso.org

[3] S. Baroni, P. Giannozzi, and E. Isaev, Reviews in Mineralogy & Geochemistry, 71:39-57 (2010)