MM 35: Topical Session Theory meets Experiment III - Bond-order Potentials and Finite

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SAPIENS, a DFT and experimental based thermophysical database for pure elements

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Steels and Ni-based superalloys are multicomponent and multiphase materials. A theoretical approach for predicting phase stability as a function of composition, temperature and pressure for these materials should use the same method for all the phases since changes in potentials, approximations, etc can introduce differences which are of the same order of magnitude of the differences in energy required to describe the stability of real alloys. We developed a consistent firstprinciples database for Helmholtz energies from which thermophysical properties such as volume, heat capacity, bulk modulus, thermal expansion, can be calculated. Our approach took into account the contribution of different excitations (phonons, electronic excitations, magnons) for the temperature dependence. The vibrational contribution was evaluated within the Quasi-Harmonic Approximation. The electronic contribution was evaluated using Fermi-Dirac statistics and DFT based electronic Density of State. Magnetism was calculated using Heisemberg hamiltonian and Quantum Montecarlo. The methodology was applied to Fe, Cr, Ni, Al pure elements. Results were compared with an extended set of experimental data.