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Ab Initio Determination of Free Energies at Finite Temperatures for High-Throughput Modeling

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The combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts has rapidly advanced over the past few years and providing now a powerful basis for high-throughput fully parameter-free schemes. Key to all these schemes is the highly accurate determination of free energies and free energy surfaces along reaction paths. In the first part of the talk recently developed concepts will be discussed that allow the computation of the temperature dependence of all free energy contributions such as electronic, harmonic, anharmonic, magnetic and structural excitations with a hitherto not achievable accuracy [1,2]. In the second part the possibilities this approach offers to describe and understand real world materials properties will be demonstrated. Examples will address the computation of *ab initio* CALPHAD data, the identification of mechanisms in modern high-strength steels and the description of chemical trends in magnetic shape memory alloys [3,4].

[1] F. Körmann, A. Dick, T. Hickel, J. Neugebauer, Phys. Rev. B **81**, 134425 (2010).
[2] B. Grabowski, L. Ismer, T. Hickel, and J. Neugebauer, Phys. Rev. B **79**, 134106 (2009).
[3] M.A. Uijttewaal, T. Hickel, J. Neugebauer, M.E. Gruner and P. Entel, Phys. Rev. Lett. **102**, 035702 (2009).
[4] B. Hallstedt, D. Djurovic, J. von Appen, R. Dronskowski, A. Dick, F. Körmann, T. Hickel, J. Neugebauer, Calphad, 129-133 (2010).