RUHR-UNIVERSITÄT BOCHUM
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Advancing *ab initio* Methods to Finite Temperatures: The Opening of New Routes in Materials Design

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Fully parameter-free *ab initio* methods based on density functional theory are steadily gaining popularity. Their atomistic view on physical processes and the access to chemical trends are attractive for a knowledge-driven development of novel electronic, biological or engineering materials. Currently, however, two problems hamper the application to a true materials design: the uncertainty about the performance of the employed exchange-correlation functionals and the apparent restriction of the method to ground state (T = 0 K) properties. For the understanding and prediction of many material properties including their phase diagrams, however, finite temperature effects are decisive and cannot be ignored. Over the last years we have therefore developed a large range of computational tools in my group to advance *ab initio* approaches towards finite temperatures. A key challenge was and is the accurate determination of free energies, considering in addition to the commonly used T = 0 K energies all possible excitation mechanisms such as electronic, vibrational, magnetic and structural excitations [1]. Within this talk I will introduce key ideas of these approaches, with the focus on the new physical insight that can be gained. Examples will address a newly discovered universal behavior of quantum corrections for magnetic excitations [2] as well as the critical and unexpected role of non-adiabatic coupling effects stabilizing certain phases [3]. The developed simulation tools provide a hitherto not achievable accuracy opening new routes to study finite temperature properties, to resolve long-standing questions in material science or to explore new strategies in materials design. Examples will include the identification of precursor effects in melting, chemical trends in the deformation behavior of modern high-strength steels, or the nature of phase transitions in magnetic shape-memory alloys [4].

[1] T. Hickel, B. Grabowski, F. Körmann, J. Neugebauer, J. Phys: Cond. Mat. **24**, 053202 (2011).
[2] F. Körmann, A. Dick, T. Hickel, J. Neugebauer, Phys. Rev. B **83**, 165114 (2011).
[3] F. Körmann, A. Dick, T. Hickel, J. Neugebauer, Phys. Rev. B **85**, 125104 (2012).
[4] M. Uijttewaal, T. Hickel, J. Neugebauer, M. Gruner, P. Entel, Phys. Rev. Lett. **102**, 035702 (2009).

Einführung: Prof. Dr. R.-J. Dettmar

Die Fakultät lädt alle Interessierten herzlich ein.

Ab 11.45 Uhr Kaffee/Tee im Hörsaal