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First principles calculations of the thermodynamics of magnetic nanoparticles using the Wang-Landau Embedded Cluster Method[1]
MARKUS EISENBACH, Oak Ridge National Laboratory, BALAZS UJFALUSSY, Research Institute for Solid State Physics and Optics, Budapest — Calculations of the ground states of magnetic nanoparticles can be performed reliably both non-relativistically as well as by solving the Dirac equation using Density Functional Theory. Here we present a method that allows us to calculate the free energy and magnetization of nanoscale systems on surfaces by combining the relativistic embeded cluster method [B. Lazarovits, L. Szunyogh, and P. Weinberger, Phys Rev B 65 (2002)] with the Wang-Landau method [F. Wang and D. P. Landau, PRL 86, 2050 (2001)]. We show results for the thermodynamic properties and finite temperature magnetization of surface nanostractures, in particular monatomic magnetic chains on surfaces.

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