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Order-disorder phase transitions: a DFT - (Wang-Landau) MC study MIRA TODOROVA, School of Physics, The University of Sydney, Australia, MIKAEL BORG, University of Toronto, Toronto, Canada, CATHERINE STAMPFL, School of Physics, The University of Sydney, Australia, MATTHIAS SCHEFFLER, Fritz-Haber-Insitut der Max-Planck Gesellschaft, Berlin, Germany
— Using a hybrid statistical mechanics method comprising the use of a Lattice-gas Hamiltonian (LGH) determined from ensity-functional theory and subsequent Monte Carlo (MC) calculations, we obtain a phase diagram for Na-Al surface alloys from first-principles and compare it to experimental results [1]. A safe approach towards parametrizing a LGH from the self-consistent evaluation of the electronic structure starts with an analytic form for the long-range pair-interactions. This expression is corrected in the short and medium range using DFT derived data, also including nearsighted many-body terms. An ensuing cross-validation is of utmost importance to ensure that the corrections (to the long-range part) are assessed with an optimum accuracy. The thus extracted LGH is used to perform MC calculations, also using the new Wang-Landau MC algorithm [2], which allows us to reliably determine the transition temperature.
[1] M. Borg *et al.*, Chem. Phys.Chem. **6**, 1923 (2005).
[2] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

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