Order-disorder phase transitions: a DFT - (Wang-Landau) MC study

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— Using a hybrid statistical mechanics method comprising the use of a Lattice-gas Hamiltonian (LGH) determined from density-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.


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