Calculation of the chemical potentials of a two-component system on the example of FeO

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The calculation of chemical potentials is a practically important problem, connected for example with phase equilibrium or with defect formation energies. In this work we consider the method of calculating the chemical potential by thermodynamic integration. The result obtained using molecular statics is compared with their direct calculations from molecular dynamics via defect formation energies [1].
Molecular dynamic calculation performed in the FeO wustite slab, which is in equilibrium with some dilute gas phase.The interatomic interaction is given by the Tersoff potential [2].

[1] Smirnov G S and Stegailov V V 2019 *Journal of Physics: Condensed Matter* **31** 235704
[2] Byggmästar J, Nagel M, Albe K, Henriksson K O E and Nordlund K 2019 *Journal of Physics: Condensed Matter* **31** 215401