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Equation of state of paramagnetic CrN from ab initio disordered local moments molecular dynamics
IGOR ABRIKOSOV, PETER STENETEG, BJÖRN ALLING, IFM, Linköping University, Sweden — A first-principles method is suggested for the calculation of thermodynamic properties of magnetic materials in their high temperature paramagnetic phase [1]. It is based on ab-initio molecular dynamics and simultaneous redistributions of the disordered but finite local magnetic moments. We apply this disordered local moments molecular dynamics (DLM-MD) method to the case of CrN and simulate its equation of state. In particular the debated [F. Rivadulla et al., Nat Mater 8, 974 (2009); B. Alling et al., Nat Mater 9, 283 (2010)] bulk modulus is calculated in the paramagnetic cubic phase and is shown to be very similar to that of the antiferromagnetic orthorhombic CrN phase for all considered temperatures.

[1] P. Steneteg, B. Alling, I. A. Abrikosov, arXiv:1110.1331v1 [cond-mat.mtrl-sci]

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