Progress in automatic quantum mechanical calculations of materials thermodynamics

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Many thermodynamic properties of materials can be automatically predicted from DFT calculations through the integrated framework AFLOW [1, 2]. We have implemented automated frameworks to calculate vibrational properties using Debye-Grüneisen models [3], or using finite displacement calculations to obtain the anharmonic interatomic force constants and the phonon modes. We have recently formulated descriptors for configurational and structural entropy based on DFT calculations for different structures and configurations [4]. These results can then be used to predict the properties, stability and synthesizability of materials at finite temperature.

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[4] E. Perim *et al.*, Nature Communications (in press) (2016). Available at arXiv:1606.01162.