Machine learning of DFT internal energies for carbon and boron structures

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Machine learning (ML) models [1–3] have become popular in the field of condensed matter physics, to solve problems which are beyond the capabilities of ab-initio techniques. An example of systems studied with ML techniques are non-periodic systems; in this case structures are represented through a Coulomb matrix [1] or bag of bonds (BoB) [4]. However, these approaches cannot be used to represent crystal structures due to practical reasons. For periodic systems, different approaches based on space groups/symmetry [5], radial distribution function [6], etc. have been used. In this work, we developed a physically motivated structure representation of crystals based on the atomic arrangement and bond orientation of the system, and used it to predict internal energies of carbon and boron structures, generated by different crystal structure prediction techniques. For our ML model, we have found that the support vector regression performs the best among different techniques.

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[1] M. Rupp et. al. *Phys. Rev. Lett.* 108, 058301 (2009)
[2] A. Grisafi et. al. *Phys. Rev. Lett.* 120, 036002 (2018)
[3] J. Behler, M. Parrinello *Phys. Rev. Lett.* 98, 146401 (2007)
[4] K. Hansen et. al. *J. Phys. Chem. Lett.* 6, 2326-2331 (2015)
[5] A. Jain et. al. *Phys. Rev. B* 98, 21 (2018)
[6] K.T. Schütt et. al. *Phys. Rev. B.* 89, 205118 (2014)