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Applications of crystallography data in force-field and density functional theory calculations: JARVIS database

Kamal Choudhary
National Institute of Standards and Technology, USA

Crystal structure information can be used to characterize material-properties using quantum density functional theory and classical force-field calculations. JARVIS database is a part of Materials Genome Initiative at National Institute of Standards and Technology (NIST) enabling users to access material property calculation data through easy web-interface. JARVIS-FF database currently consists of 3248 entries including energetics and elastic property calculations and it is still increasing. We also include computational tools for convex-hull plots for DFT and FF calculations. The data covers 1471 materials and 116 force-fields. A major feature of this database is that the web interface offers easy look up tables to compare at a glance the results from different potentials (for the same system). In addition, both the complete database and the software coding used in the process have been released for public use online. JARVI-DFT database consists of more than 5000 DFT calculations for three-dimensional (3D) bulk and single layer 2D materials data for structural, electronic and elastic properties. We use lattice-constant criteria to identify potentially novel 2D materials. We predicted at least 1485 2D materials based on relative error in lattice constants obtained from semi-local DFT and Inorganic Crystal Structure Database (ICSD) data. We calculate exfoliation energy as a verification of our lattice-constant criteria.

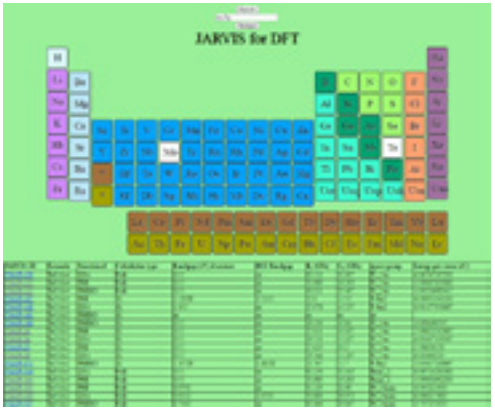

Figure-1: JARVIS database online

Biography

Kamal Choudhary has expertise in molecular dynamics, density functional theory and machine-learning based calculations. He has built JARVIS database at NIST to enable users access classical and quantum mechanical data of material free of cost to enable future materials discovery. He was graduated with PhD in Materials Science and Engineering from University of Florida in 2015 under the guidance of Dr. Susan B Sinnott.

kamal.choudhary@nist.gov

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