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High-throughput identification and characterization of two-dimensional materials using density functional theory

Kamal Choudhary and **Francesca Tavazza**
National Institute of Standards and Technology, USA

We introduce a simple criterion to identify two-dimensional (2D) materials based on the comparison between experimental lattice constants and lattice constants mainly obtained from Materials-Project (MP) density functional theory (DFT) calculation repository. Specifically, if the relative difference between the two lattice constants for a specific material is greater than or equal to 5%, we predict them to be good candidates for 2D materials. We have predicted at least 1356 such 2D materials. For all the systems satisfying our criterion, we manually create single layer systems and calculate their energetics, structural, electronic, and elastic properties for both the bulk and the single layer cases. Currently the database consists of 1012 bulk and 430 single layer materials, of which 371 systems are common to bulk and single layer. The rest of calculations are underway. To validate our criterion, we calculated the exfoliation energy of the suggested layered materials, and we found that in 88.9% of the cases the currently accepted criterion for exfoliation was satisfied. Also, using molybdenum telluride as a test case, we performed X-ray diffraction and Raman scattering experiments to benchmark our calculations and understand their applicability and limitations.

Biography

Kamal Choudhary is a Post-doctoral Researcher at National Institute of Standards and Technology. His current area of research is database development and management for atomistic calculation using classical force-field, quantum density functional theory and machine learning through JARVIS (Joint Automated Repository for Various Integrated Simulations) project.

kamal.choudhary@nist.gov