JARVIS: High Throughput Classical and Quantum Calculation Database for Materials

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**JARVIS-FF: Classical**

\[ F = ma = -\nabla V(r) \]

- Approximations for V (force-fields): EAM, EIM, MEAM, AIREBO, REAXFF, COMB, COMB3, TERSOFF, SW etc.
- Goal of JARVIS-FF:
  - Evaluation of classical force-fields and provide easy user-interface,
  - Comparison with DFT and experimental data
  - Providing all the input files
- Current status:
  - 3583 calculations (>19000 sub-calculations) with LAMMPS
  - Version 1: Energetics, convex hull, elastic constants calculation
  - Version 2: Addition of visualization of structure, vacancy formation energies, surface energies, phonon density of states and phonon band structure, visualization of phonons (under development phase)
  - Now integrated in LAMMPS official website

**JARVIS-DFT: Quantum**

\[ H \psi = E \psi \]

- Approximations for Vxc (Exchange-correlation): LDA, PBE, vdW-DF, Hybrid etc.
- Goal of JARVIS-DFT:
  - Identification of 2D bulk and multi-layer, Solar and Thermoelectric materials out of thousands of materials from databases
  - Characterizing their properties
  - Other DFT databases uses constant k-point, energy cut-off and PBE functionals, not suitable for 2D materials, we use vDw-DF
  - Providing all the input files
  - Effect of XC on properties
- Current status: (under development phase)
  - 873 calculations (>25000 sub-calculations) with VASP

**Easy Web-interface**

- [JARVIS for Force-fields](http://www.ctcms.nist.gov/~knc6/JAVSforcefields.html)
- [JARVIS for DFT](http://www.ctcms.nist.gov/~knc6/JAVSFortran.html)

**Implementation of Machine Learning Tools**

- Relative error in \( C_{ij} \)
- PCA analysis

**Ongoing work**

- JARVIS-ONE: Tools to accumulate and compare various DFT, FF and experimental data in one web-interface
- JARVIS-FF: Thermal conductivity, genetic algorithm evaluation, stacking fault, grain-boundary energies calculations
- JARVIS-DFT: 2L, 3L, 4L structures for 2D materials, comparison of solar cell material and thermoelectric properties performance, HSE band-structures calculations
- Implementation of voice-recognition based query tools and better machine learning tools

**Acknowledgment**

Thanks to:
- Simon R. Phillip, University of Florida,
- Susan B. Sinnott, Pennsylvania State University,
- Karelyn E. Campbell and Zachary T. Traut, NIST,
- Kristin Persson and Joseph Montoya, LBNL for helpful discussions