Title: DFT Benchmarking

Contact: Dr. Francesca Tavazza, [francesca.tavazza@nist.gov](mailto:francesca.tavazza@nist.gov)

Contributors: Joshua J. Gabriel, Faical Y. Congo, Alex Sinnott, Thomas C. Allison, Francesa Tavazza, Richard G. Hennig

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Manifest:

* Pade.csv
* Precs.csv
* README.txt

Description:

All the data in this project are generated running Density Functional Theory (DFT) simulation either on NIST computer clusters of through our collaborators at University of Florida. The final data consist in relaxed atomic structures and corresponding energetic, structural (equilibrium lattice constants) and mechanical properties (bulk modulus and bulk modulus pressure derivative). The metadata consist in the initial and relaxed structures, the description of the code, of the k points and of all the parameters used in running the simulations (energy or real space cutoff, type of minimization, occupation, etc.).

Pade.csv: provides the Pade extrapolates at infinite k-point of the materials properties for transition metals in stable and metastable structures: Volume per atom (V0), Bulk Modulus (B) and Bulk Modulus Pressure Derivative (B'). All results are obtained from DFT calculations performed with the PBE GGA exchange correlation functional in two codes: VASP and DMol3 and the LDA exchange correlation functionals of PW92 (DMol3) and PZ81 (VASP).

Precs.csv: provides the numerical precisions of DFT calculated material properties for transition elements: Equilibrium Volume per atom (V0), Bulk Modulus (B) and the Bulk Modulus Pressure Derivative (dB/dP) as a function of the kpoints density chosen for two codes VASP and DMol3. We use the GGA exchange correlation of PBE in VASP and DMol3 and the LDA exchange correlation of PZ81 in VASP and PWC in DMol3. We calculate the numerical precision using the Pade extrapolates of the material properties (Pade.csv).

The two CSV files are also available at:

<https://researchdata.nist.gov/Materials-/Pade-Extrapolates-of-Material-Properties-from-DFT-/ak25-uy3p>

<https://researchdata.nist.gov/Materials-/Numerical-Precision-of-Material-Properties-from-DF/ej74-7uwn>