VASPLAB v0.6

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VASPLAB is a set of MATLAB scripts that allow various output files of the Vienna ab inito simulation package (VASP) to be read into MATLAB. There are also some other utilities

To install VASPLAB, place the VASPLAB folder somewhere on your hard drive (such as in your MATLAB folder). Then, from MATLAB, open File→Set Path, and add the VASPLAB folder to your path.

Below is a summary of VASPLAB functions. See the MATLAB documentation for more information (for example, by using the command `help import_poscar`).

`atomic_radius(Z)`
Get atomic radius of element.

`chemsym2number(symbol)`
Get the atomic number for a chemical symbol.

`export_df3(filename,chg)`
Export volumetric data as a DF3 file.

`export_poscar(filename,geometry)`
Export a geometry struct as a VASP POSCAR file.

`fit_murnaghan_eos(V,E)`
Fit to the Murnaghan equation of state.

`hyperdistance(geometry1,geometry2)`
Calculate hyperdistance between two geometry structures.

`import_chgcar(filename)`
Import a VASP CHGCAR file.

`import_doscar(filename)`
Import a VASP DOSCAR file.

`import_eigenval(filename)`
Import a VASP EIGENVAL file.

`import_locpot(filename)`
Import a VASP LOCPOT file.

`import_oszicar(filename)`
Import energies from a VASP OSZICAR file.

`import_outcar(filename,param)`
Import data from a VASP OUTCAR file.

`import_poscar(filename)`
Import a VASP POSCAR/CONTCAR file.

`interpolate_poscar(filename1,filename2,N)`
Interpolate a chain of images between two POSCAR files.

`jmol_color(Z)`
Get color assigned to an element.

`kpath_length(k,A,mode)`
Find the distance along a path in k-space.

`murnaghan_eos(V,x)`
Evaluate the Murnaghan equation of state.

`neb_energies(directory)`
Extract energies and hyperdistance from NEB calculation.

`neb_spline(directory,N)`
Fit energies and forces of a NEB calculation using a spline.

`num_images()`
Determine number of images used in a NEB calculation.

`number2chemsym(Z)`
Get the chemical symbol for an atomic number.

`permute_coords(geometry1,geometry2)`
Permute ions in a geometry to match another geometry.

`plot_neb_spline(directory)`
Plot the energy along a NEB path.

`reciprocal_lattice(A)`
Find the reciprocal lattice.

`supercell(geometry1,array)`
Create a supercell by replicating a geometry.

`vasp_xml(filename,param)`
Import data from a vasprun.xml file.