Interfacing abinit with external libraries or packages: electronic structure analysis and molecular dynamics

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In this talk, I will present our efforts in interfacing Abinit with two different packages.

PyProcar is a robust, open-source Python library used for pre and post-processing of electronic structure data from DFT calculations. The PROCAR file generated from DFT calculations contain the projections of the Kohn-Sham wave functions for every energy band and k-point for all the atoms in the structure also taking spin into account. PyProcar parses the energy band structure and the orbital resolved contributions and provides a set of graphical analysis including the electronic band structure with orbital, atom and spin projection, spin-texture, 3D and 2D Fermi surface with orbital, atom, spin and Fermi velocity projection, multi-band comparison, band unfolding to name a few.

Molecular Dynamics with Constraints (mdwc) package is an open source, user friendly Python program to perform constrained molecular dynamics simulations. It utilizes the Rahman-Parrinello Lagrangian to perform NPT and NVT calculations. Based on the SHAKE algorithm, mdwc can impose constraints on bond distances, angles, atomic positions, lattice parameters, angles between lattice vectors and the volume of the unit cell. Libraries from this development can be linked directly to any software that provides forces and energies. While the molecular dynamics code propagates the particles in the simulation, the energy and forces are calculated through Abinit. These calculations can be easily performed with the help of a clear set of Jupyter notebook examples.