## O.8   Interfacing electronic structure codes for band structure, Fermi surface and Elastic analysis

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In this talk we will present the most recent developments into the pre/processing code **PyProcar** and the mechanical and elastic property analysis tool **MechElastic**. PyProcar is capable of performing a multitude of tasks including plotting plain and spin/atom/orbital projected band structures, unfolding bands of a super cell and plotting partial density of states and supports DFT codes such as Abinit, VASP, Quantum Espresso, Elk and Lobster. Recent developments in PyProcar mainly revolves around enhancements to its 3D Fermi surface implementation and 2D Fermi projection. Users have access to generating Fermi surfaces with atom, orbital and spin projections. Moreover, provided external momentum dependent quantities such as Fermi velocity and electron-phonon coupling, PyProcar is able to project them onto a Fermi surface providing a comprehensible graphical representation. Plotting Wannier interpolated Fermi surfaces calculated from the wannier90 library is supported through PyProcar bxsf parser. Our package allows to obtain Fermi surfaces from primitive cells and projected in the unit cell. Cross-sectional slicing of the Fermi surface has also been added, allowing users to investigate 2D cross sections. Additional Fermi surface properties such as surface area, curvature and effective mass are also obtainable. On the other hand, MechElastic calculates mechanical and elastic properties of bulk and 2D material including elastic moduli, melting temperature, Debye speed and temperature, elastic wave velocities, elastic anisotropy, mechanical stability based on the elastic tensor read from the DFT codes Abinit, VASP and Quantum Espresso and further facilitates generating 2D and 3D visualizations of these properties through an interface with the ELATE package. Additionally, MechElastic performs Equation of State (EOS) analysis through popular EOS models. The EOS function further calculates the possible phase transition paths for different phases of a material and displays this information as a directed graph plot.