PyProcar: A Python library for electronic structure pre/post-processing

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The PyProcar Python package plots the band structure and the Fermi surface as a function of site and/or s,p,d,f - projected wavefunctions obtained for each k-point in the Brillouin zone and band in an electronic structure calculation. This can be performed on top of any electronic structure code, as long as the band and projection information is written in the PROCAR format, as done by the VASP, ABINIT and ELK codes. PyProcar can be easily modified to read other formats as well. This package is particularly suitable for understanding atomic effects into the band structure, Fermi surface, spin texture, etc. PyProcar can be conveniently used in a command line mode, where each one of the parameters define a plot property. In the case of Fermi surfaces, the package is able to plot the surface with colors depending on other properties such as the electron velocity or spin projection. The mesh used to calculate the property does not need to be the same as the one used to obtain the Fermi surface. A file with a specific property evaluated for each k-point in a mesh and for each band can be used to project other properties such as electron–phonon mean path, Fermi velocity, electron effective mass, etc. Another existing feature refers to the band unfolding of supercell calculations into predefined unit cells.