MedeA Fermi Surface

Living on the Edge

At-a-Glance

MedeA®[1] *Fermi Surface* displays isosurfaces of electronic energies of metals, semiconductors, and insulators in k-space, and lists the effective masses of all bands at arbitrary k-points.

Key Benefits

- Straightforward setup of the calculation
- Automated distribution over a large number of tasks enables quick calculation
- Easy selection of isosurface energy and isosurface sheets for display
- Access to effective masses of all bands at any k-point

Allan Mackintosh's suggestion to define a metal as 'a solid with a Fermi surface' underlines the importance of this quantity for a deeper understanding of materials' properties[2]. It reflects the outstanding contribution electrons at (and within an energy range of k_BT of) the Fermi surface make to a materials transport properties. In addition, the Fermi surface plays a paramount role in determining electronic system's response to external perturbations and in indicating instabilities arising from interaction with the electrons' spins or the vibrational degrees of freedom.

MedeA Fermi Surface thus provides ample insight into the 'life on the edge'[3]. Since this 'edge' can be shifted, even the isosurfaces at the full spectrum of metals and semiconductors are accessible with MedeA Fermi Surface.

As a simple example, the Fermi surface of Cu as shown in the below figure closely resembles the perfect spherical Fermi surface of a free electron band, but shows distinct deviations in the form of necks opening along the <111> directions. This is due to band distortions at the Brillouin-zone boundaries, caused by the real crystal potential. In general, calculated Fermi surfaces have a very high predictive power, and while confirming experimentally determined Fermi surfaces, *e.g.*, by de Haas-van Alphen measurements or angle-resolved photoemission spectroscopy, facilitate interpretation of these data[4].

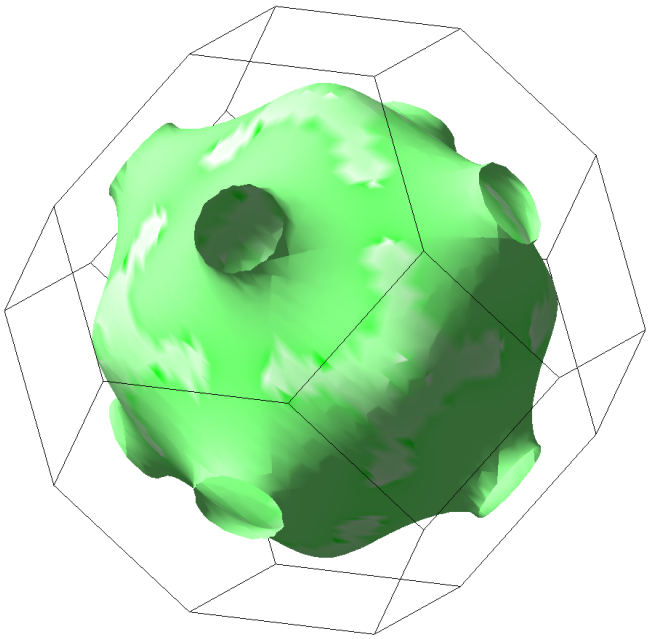

Figure 1: Fermi surface of Cu as calculated using MedeA Electronics.

The Fermi surface is the stage on which the "drama of the life of the electron" is played out.

M. I. Kaganov and I. M. Lifshits, "Electron theory of metals and geometry", Sov. Phys. Usp. 22, 904 (1979)

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] A. R. Mackintosh, "The Fermi surface of metals", Sci. Am. **209**, 110 (1963) (DOI)

[3] S. B. Dugdale, "Life on the edge: a beginner's guide to the Fermi surface", Phys. Scr. **91**, 053009 (2016) (DOI)

[4] Th. Straub, R. Claessen, P. Steiner, S. Hüfner, V. Eyert, K. Friemelt, and E. Bucher, "Many-body definition of a Fermi surface: Application to angle-resolved photoemission", Phys. Rev. B **55**, 13473 (1997) (DOI)

Key Features

- An intuitive user interface allows completely automated setup, execution, and processing of the background jobs required to calculate isosurfaces of the electronic energies and the corresponding effective masses
- Compute electronic eigenvalues with MedeA VASP
- Apart from the calculational parameters of the underlying MedeA VASP calculation, MedeA Fermi Surface requires only specification of the fineness of the **k**-point grid used to display the isoenergy surfaces
- Take advantage of MedeA's robust JobServer and TaskServer Infrastructure with full integration into the MedeA Environment of the MedeA's robust JobServer and TaskServer Infrastructure
- Efficiently manage calculations in line with the computational resources
- Automatically detect and use space-group symmetry

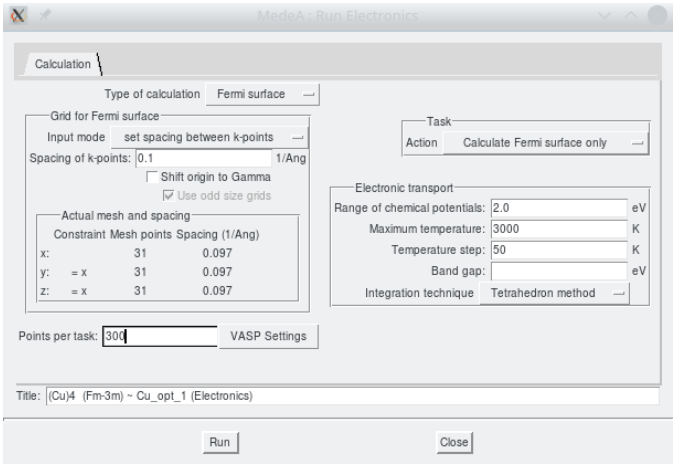

Figure 2: MedeA Fermi Surface Screenshot: Graphical user interface controlling setup of the calculation

Properties

- Three-dimensional isosurfaces of electronic energies (Fermi surfaces) in **k**-space
- Interactive analysis of effective masses for each band at any point in **k**-space
- Interpolated electronic band structure displayed for orientation

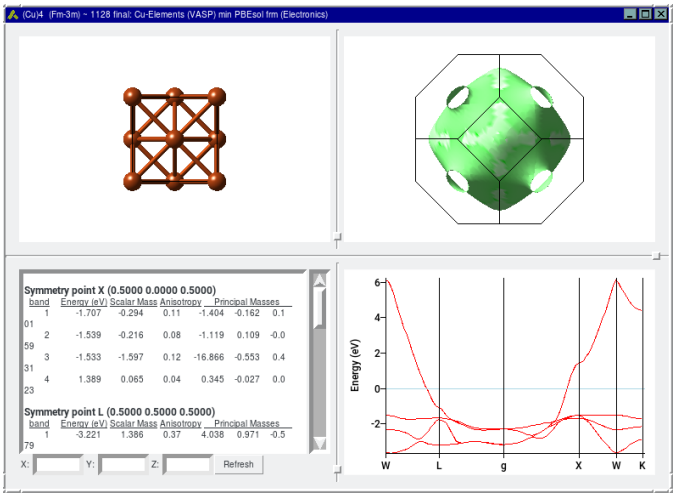

Figure 3: MedeA Fermi Surface Screenshot: Graphical user interfaces for the display and analysis of calculated Fermi surfaces and effective masses

Required Modules

- *MedeA Environment*
- *MedeA VASP*

Related Modules

- *MedeA Electronics*

Find Out More

Check out the closely related datasheet on MedeA Electronic Transport.

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