

# MedeA *Fermi Surface*

Living on the Edge

## At-a-Glance

*MedeA*<sup>1</sup> *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<sup>2</sup>. It reflects the outstanding contribution electrons at (and within an energy range of  $k_B T$  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'<sup>3</sup>. 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  $\langle 111 \rangle$  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<sup>4</sup>.

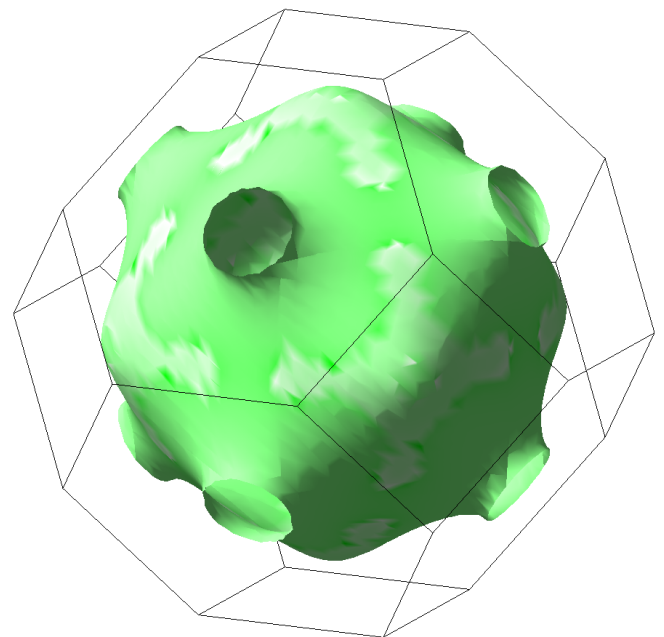


Figure 1: Fermi surface of Cu as calculated using *MedeA Electronics*.

*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)

<sup>1</sup> MedeA and Materials Design are registered trademarks of Materials Design, Inc.

<sup>2</sup> A. R. Mackintosh, "The Fermi surface of metals", *Sci. Am.* **209**, 110 (1963) (DOI)

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

<sup>4</sup> 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  $\mathbf{k}$ -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

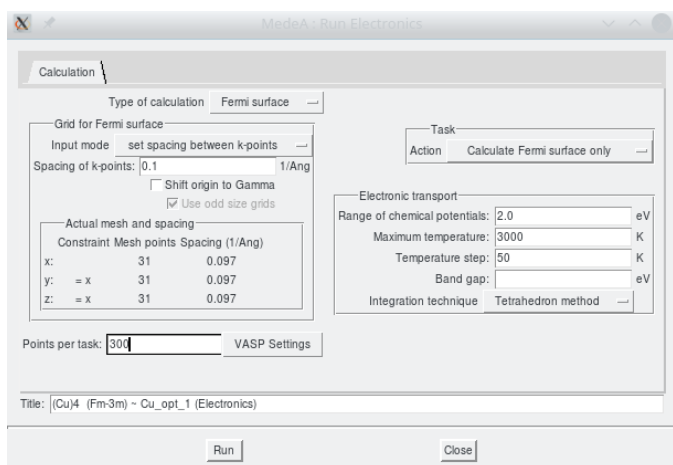


Figure 2: MedeA Fermi Surface Screenshot: Graphical user interface controlling setup of the calculation

## Properties

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

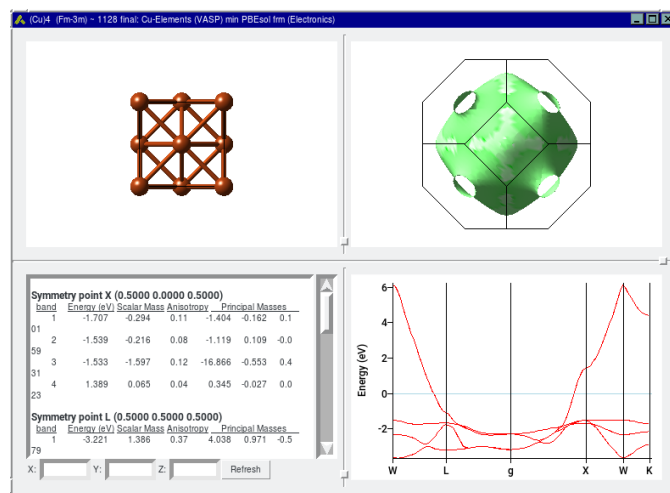


Figure 3: MedeA Fermi Surface Screenshot: Graphical user interfaces for the display and analysis of calculated Fermi surfaces and effective masses

## Required Modules

- MedeA Environment
- MedeA VASP

## Related Modules

- MedeA Electronics

## Find Out More

Check out the closely related datasheet on [MedeA Electronic Transport](#).