



MedeA Electronics

What the electrons at the Fermi sea can tell us

At-a-Glance

MedeA^{®1} Electronics computes key electronic properties of metals, semiconductors, and insulators including isoenergy (Fermi) surfaces, electronic contributions to the electrical and thermal conductivity, thermoelectric power, and effective masses.

Key Benefits

- Straightforward setup of the calculation and automated distribution over a large number of tasks
- Easy selection of isosurface energy and isosurface sheets for display
- Transport quantities displayed as a function of temperature, chemical-potential shift (rigid-band doping), or carrier density
- Adaptation of fundamental band gap for refined calculation of transport properties

Due to the Pauli principle, only the electronic states at the Fermi energy, and within a narrow energy range of width $k_B T$ around it, govern a material's response to external electric or magnetic fields, or temperature gradients. Thus insight into the energy distribution of these states, and the nature of their wave functions thus is of utmost importance for understanding the material's properties.

MedeA Electronics explores the electronic states within a narrow energy range about the Fermi energy, by giving access to ground-state properties, such as Fermi surfaces, specific heats, and effective masses, as well as transport properties, like the electronic contributions to the electrical and thermal conductivities and the thermoelectric power.

For example, the Fermi surface of MoO_2 , as shown in the Figure below, identifies three different sheets, namely, an electron-like peanut-shaped Fermi surface centered at the Γ point and two smaller hole-like Fermi surfaces each centered at

the Y point, explaining the anisotropic electrical conductivity. Both angle-resolved photoemission spectroscopy and de Haas-van Alphen measurements show very good agreement with calculated Fermi surfaces, and thus underline the predictive power of first-principles calculations².

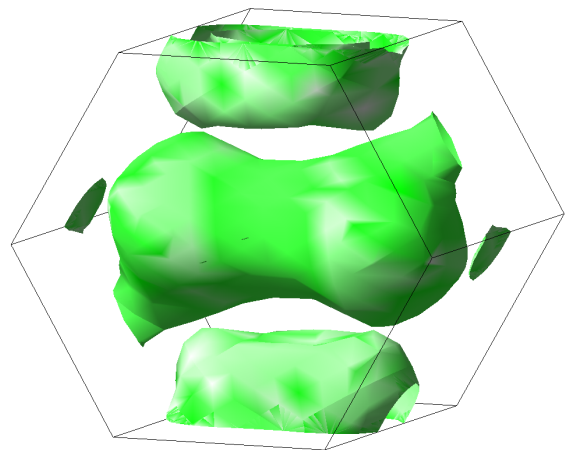


Figure 1: Fermi surface of MoO_2 calculated using MedeA Electronics

The concept of effective masses has gained importance in describing the response of electrons (and holes) to external electric and magnetic fields. Effective masses are determined by the curvature of the bands near the Fermi energy in metals or the bands close to the valence band maximum and conduction band minimum in semiconductors. Given the electronic states in that energy region effective masses can thus be straightforwardly calculated. As an example, calculated effective masses of silicon's hole and electron states are given in the following table and found in almost perfect agreement with experimental data.

² J. Moosburger-Will, J. Kündel, M. Klemm, S. Horn, P. Hofmann, U. Schwingenschlögl, and V. Eyert, Phys. Rev. B **79**, 115113 (2009) (DOI)

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

Table 1: Measured and calculated effective hole and electron masses of silicon at the valence band maximum at the Γ -point and at the conduction band minimum at $(0.43, 0.43, 0.0)$, respectively

	Exp. ³	Exp. ⁴	MedeA
Electrons			
Long Eff. Mass	0.92	0.98	0.94
Trans Eff. Mass	0.19	0.19	0.20
DOS Mass	1.06	1.08	1.09
Conductivity Mass		0.26	0.27
Heavy Hole			
Eff. Mass	0.54	0.49	0.67
Light Hole			
Eff. Mass	0.15	0.16	0.13
Split-off Band			
Eff. Mass	0.23	0.24	0.22

Deviations are observed for the heavy-hole mass, which are related to the strong anisotropy of the Γ -point hole states as nicely demonstrated in the figure below illustrating the isosurface of the electronic states of Si at 0.7 eV below the valence band maximum.

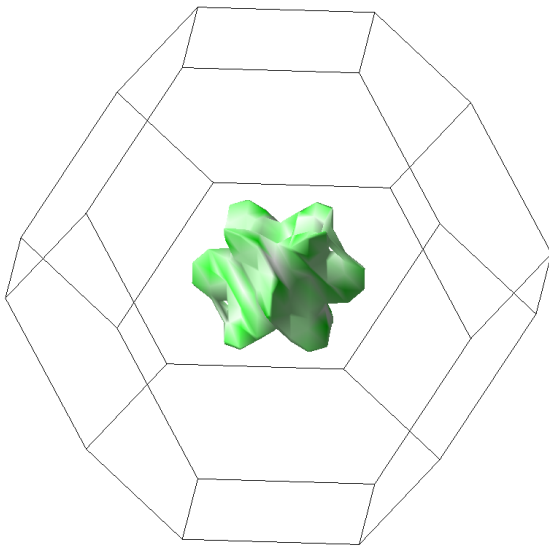


Figure 2: Isoenergy surface of Si at -0.7 eV calculated using MedeA Electronics

Key Features

- Automated setup, execution, and processing of background jobs through an intuitive user interface to calculate properties

³ H. D. Barber, Solid State Electronics **10**, 1039 (1967) (DOI)

⁴ <https://www.ioffe.ru/SVA/NSM/Semicond/Si/bandstr.html>

- Full integration in the *MedeA Environment* takes advantage of *MedeA's* robust JobServer and TaskServer Infrastructure
- Efficient management of calculations across the desired number of CPU cores
- Electronic eigenvalues computed with *MedeA VASP*
- Automatic detection and use of space-group symmetry

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
- Highly accurate effective mass tensors for selected electron or hole bands at requested points in **k**-space
- Electrical conductivity, thermal conductivity
- Thermoelectric power (Seebeck coefficient)
- Electronic specific heat
- Pauli paramagnetic susceptibility
- Hall coefficient

Value of Integration

Required Modules

- MedeA Environment*
- MedeA VASP*

Find Out More

Learn more about *MedeA Electronics* by checking out the following on Materials Design Application Notes page:

- Thermoelectric Properties of Bi_2Te_3 as calculated using *MedeA Electronics*.

Check out the Datasheets on *MedeA Fermi Surface* and *MedeA Electronic Transport* for additional information.

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com

materialsdesign.com



materials design