MedeA Electronics

What the electrons at the Fermi sea can tell us

At-a-Glance

MedeA®[5] *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_BT 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 calculations[6].

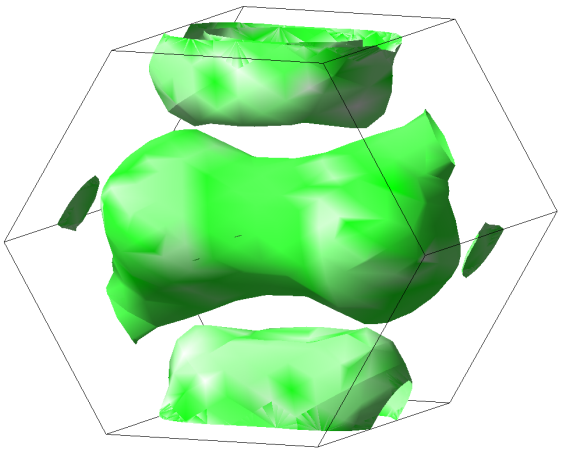

Figure 1: Fermi surface of MoO_2 calculated using MedeA Electronics

Calculated effective masses of silicon's hole and electron states of given in the following table likewise agree almost perfectly with experimental data.

Table 1: Measured and calculated Γ-point effective masses of silicon

	Exp.[3]	Exp.[4]	*MedeA*
Electrons			
Long Eff. Mass	0.98	0.98	0.96
Trans Eff. Mass	0.19	0.19	0.19
DOS Mass	1.08	1.08	1.08
Conductivity Mass	0.26	0.26	0.26
Light Hole			
Eff. Mass	0.16	0.16	0.18
Split-off Band			
Eff. Mass	0.29	0.24	0.23

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

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

[3] http://ecee.colorado.edu/~bart/book/effmass.htm'

[4] http://www.ioffe.rssi.ru/SVA/NSM/Semicond/Si/bandstr.html'

In addition, the strong anisotropy of the Γ-point hole states is nicely demonstrated in the figure below, which illustrates the isosurface of the electronic states of Si at 0.7 eV below the valence band maximum.

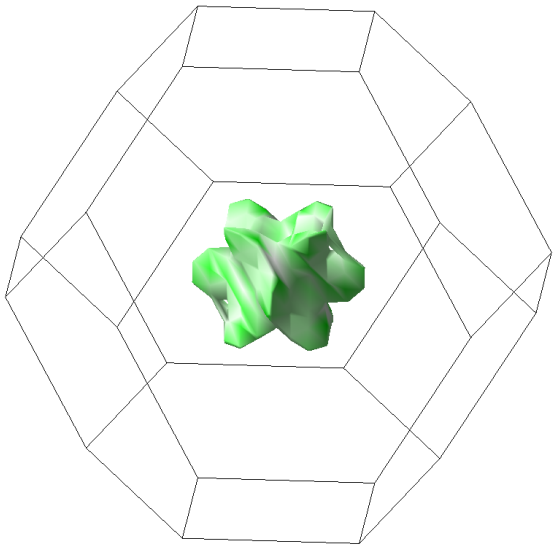

Figure 2: Isoenergy surface of Si at -0.7 eV calculated using MedeA Electronics

Key Features

- Automated setup, execution, and processing of background jobs through an intuitive user interface to calculate properties
- 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_3as calculated using *MedeA Electronics*.

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

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