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MedeA®-Electronics

MedeA®-Electronics provides the ability to calculate the electronic properties of solids that involve the electronic states in a narrow energy range about the Fermi energy, that is, those states that can be thermally activated or activated by doping. These electronic states govern the response of the material to external electric fields or temperature gradients, which produce electric and heat currents. Properties of prime interest are effective masses, electrical conductivity and thermoelectric power which complement the calculation of accurate electronic band structures using MedeA®-VASP - all of which are accessible from MedeA®-Electronics.

Key Benefits of MedeA®-Electronics

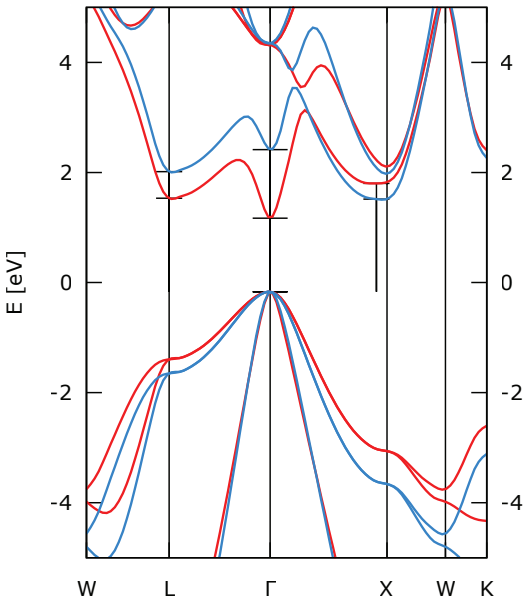
- *Predicts effective masses of electrons and holes for selected bands at requested k-points*
- *Predicts key properties of electric and heat transport as well as thermoelectricity such as the electric and thermal conductivity and thermoelectric power*

Properties from MedeA®-Electronics

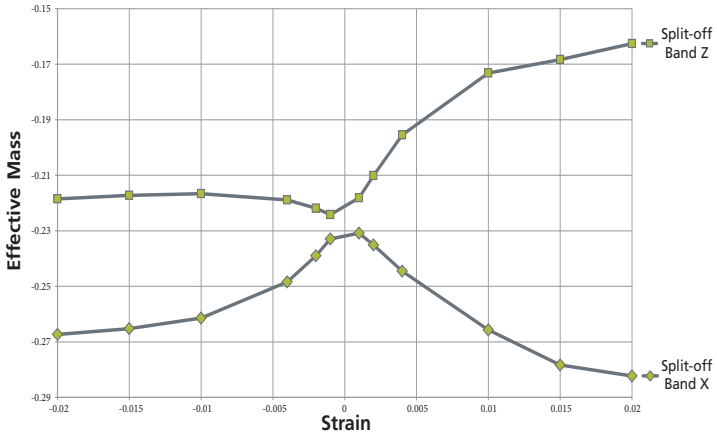
- *Highly accurate effective mass tensors for selected electron or hole bands at requested points in k-space*
- *Electric conductivity*
- *Thermoelectric power (Seebeck coefficient)*
- *Electronic contribution to thermal conductivity*
- *Hall coefficient*
- *Electronic specific heat*
- *Pauli paramagnetic susceptibility*
- *Three-dimensional rendering of isoenergy (Fermi) surfaces*
- *Exploration of the effect of doping on the isoenergy (Fermi) surface*
- *Interactive analysis of effective masses and electron velocities for each band at any point in k-space*

Required MedeA® Modules

- *Core MedeA® Environment*
- *MedeA® JobServer and TaskServer*
- *MedeA®-VASP*



Electronic band structure of GaAs calculated at the equilibrium lattice constant (5.67 Å, red) and under pressure (5.4 Å, blue). Note the change from a direct to an indirect band-gap semiconductor.



Γ-point effective masses of the split-off conduction band of Silicon under <001> strain

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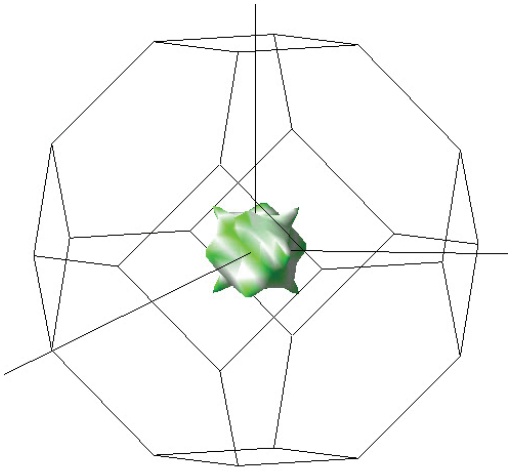
Measured and calculated Γ-point effective masses of silicon

	Exp. [1]	Exp. [2]	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
Heavy Hole			
Eff. Mass	0.49	0.49	
Light Hole			
Eff. Mass	0.16	0.16	0.18
Split-off Band			
Eff. Mass	0.29	0.24	0.23

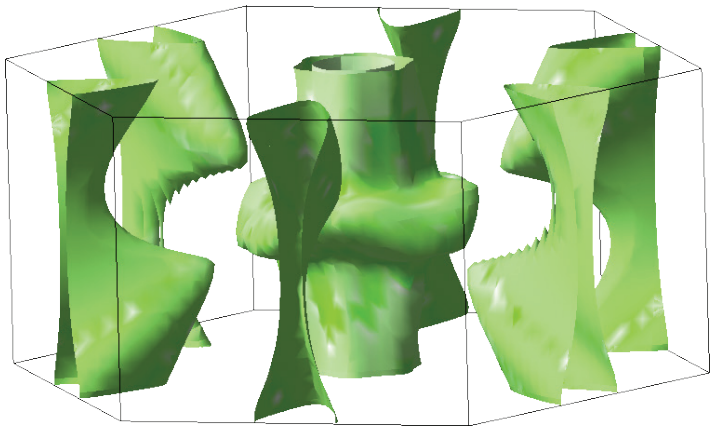
Exp [1] http://ecee.colorado.edu/~bart/book/effmass.htm
Exp [2] http://www.ioffe.rssi.ru/SVA/NSM/Semicond/Si/bandstr.html

Calculated effective masses of both hole and electron states nearly perfectly agree with experimental data. Furthermore, principle difficulties in measuring and calculating the Γ-point heavy-hole mass are easily traced to the strong anisotropy of the respective band close to this point using visualized isoenergy surfaces of silicon (Fermi surfaces of doped silicon).



Fermi surface of hole-doped silicon demonstrating the strong anisotropy of the heavy-hole band at the Γ-point

The complex multi-sheet Fermi surface of $TiTe_2$ is shown below. $TiTe_2$ is a hexagonal layered compound with Te-Ti-Te sandwiches separated by a van der Waals gap and has a complicated band structure near the Fermi energy. The strongly deformed tubes in the Fermi surface reflect the two-dimensionality of the compound as well as the strong Ti-Te bonding. A low level of doping will cause large changes in the Fermi surface and may, for example, change the electrical conductivity from two to three dimensions.



Comprehensive Analysis Suite

The combination of electronic band structures obtained from MedeA®-VASP and the properties predicted by MedeA®-Electronics gives users a toolbox for the comprehensive analysis and understanding of the electronic properties of desired materials.

MedeA®-Electronics is fully integrated into the MedeA® Environment allowing it to take advantage of the robust MedeA® JobServer and TaskServer Infastructure. Calculations are efficiently managed across the desired number of CPU cores.

Computational Characteristics

- *An intuitive user interface allows completely automated setup, execution and processing of background jobs required to calculate the above properties*
- *Eigenvalues computed with MedeA®-VASP*
- *Automatic detection and use of space-group symmetry*

For further information, visit our website www.materialsdesign.com or contact us directly as given below.

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