

A Database of Fermi Surfaces in Virtual Reality Modeling Language

We have built a database of Fermi surfaces in Virtual Reality Modeling Language (VRML) for 45 elemental solids. Running any of the free VRML browsers on an entry level personal computer, a user can rotate and fly through the 3-dimensional Fermi surfaces in real time. The homepage of the database contains a periodic table that links to the Fermi surface pages of individual elements. For each of the solids, the Fermi surface of a band that crosses the Fermi level is contained in one of the 167 VRML 1.0 files. The average size of the files is less than 70kB. An interactive version of the Fermi surfaces in VRML 2.0 format is also provided for each element. For users with high speed and high bandwidth computers, a high resolution version is also provided for each Fermi surface. The website also provides a CGI script which returns the Fermi surfaces in VRML using user-submitted energy data. Stereographic display using GIF and Java3D are also available.

Method

***ab initio* band structures is fitted to obtain tight-binding parameters.**

(e.g. D.A. Papaconstantopoulos.)

Tight-binding parameters

Diagonalization

(To generate high resolution VRML files, up to $160 \times 160 \times 160$ k-points are needed for each Brillouin zone. It took a few days for a cluster of 20 Sun Ultra 300 CPUs to complete the calculations.)

$E(k)$, ME/Mk

Isosurface code

(The code is written specially for generating Fermi surface and clipping the surfaces by Brillouin zone boundaries.)

Fermi surface in VRML 1.0 format

Adding VRML 2.0 interactive controls and coloring surfaces.

Fermi surface in VRML 2.0 format

Fermi surface in VRML 1.0 format

VRML Player
(e.g. Cosmos Player)

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Java3D display code

Platform independent display

Stereographic display

