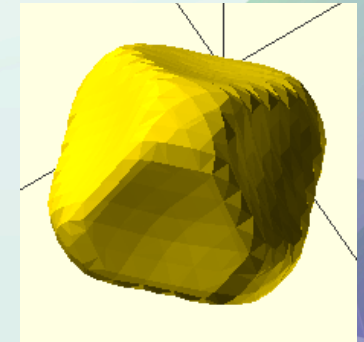
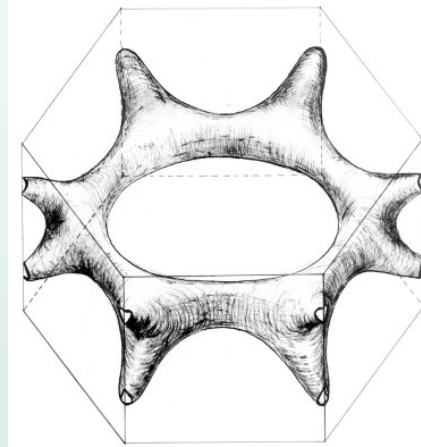
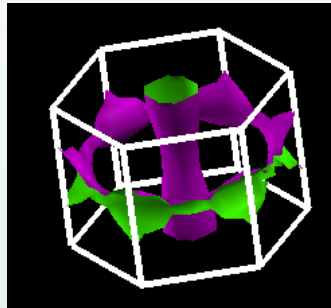
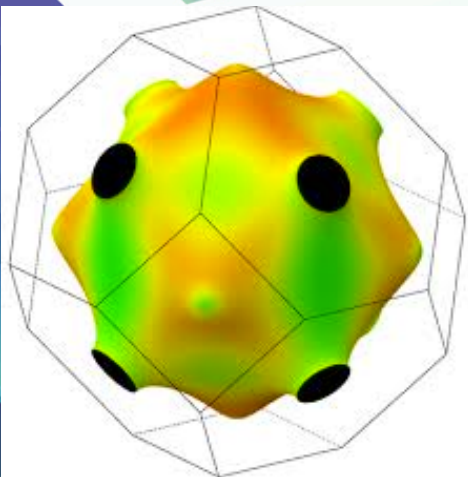


1 Dec 2015



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Firmi: get a firm grasp on your Fermi surface!



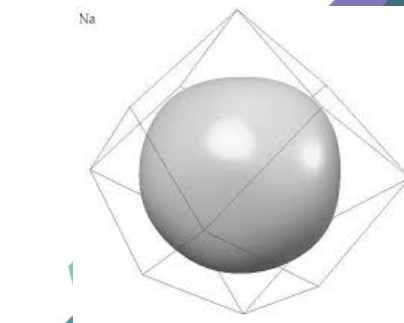
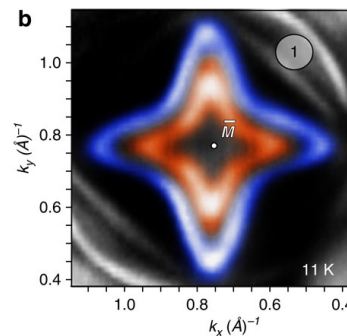
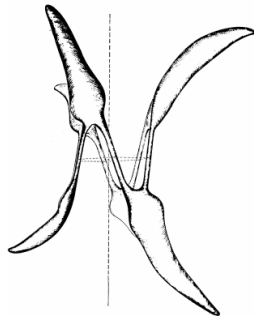
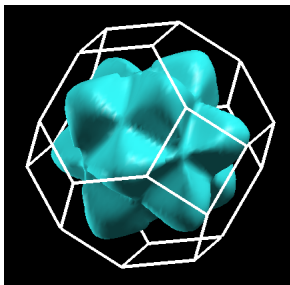
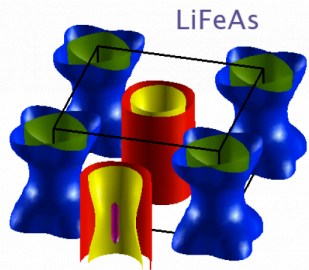
Team Name & Introduction



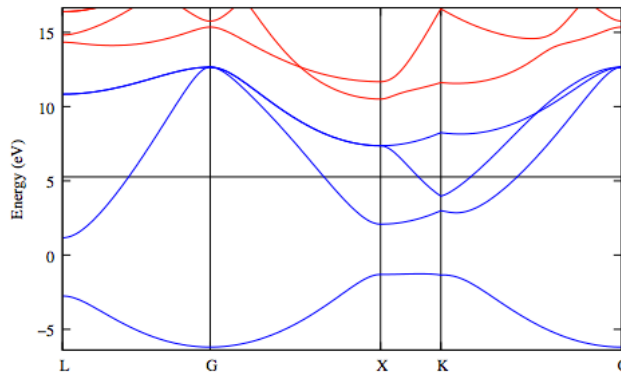
Firmi: utility to prepare a Fermi surface for 3D printing

Dr. David Strubbe, Dept. of Materials Science and Engineering, Massachusetts Institute of Technology

Dr. Ryan Cooper, Materials Science and Technology Division, Oak Ridge National Laboratory

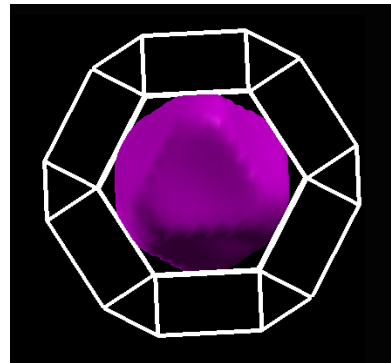


Problem Description



Key property of metals, e.g. Pb

$$\left\{ \vec{k} \mid \epsilon(\vec{k}) = \epsilon_F \right\}$$



Dividing surface in reciprocal space between occupied and unoccupied states

Important for conductivity, superconductivity, doping, electron-phonon interactions, many-body physics

Can be determined theoretically (electronic structure) and experimentally (ARPES, de Haas-van Alphen effect, etc.)

How to visualize?
tangible model!

Live Demo/Run-Through



1. Obtain 'bxsf' from an electronic structure calculation, *e.g.* Quantum ESPRESSO, Wannier90, etc. (in XCrySDen Fermi surface file format)
2. Run 'bxsf2scad.x' producing 'bxsf.scad'.
Open in OpenSCAD software.
3. In OpenSCAD menu, Design->Compile, then Design->Compile and Render (CGAL) [may take a while!].
4. In OpenSCAD menu, File->Export->STL to save file.
5. Open STL file in (*e.g.*) MakerBot software, adjust size, rotation, position.
6. Print, and enjoy!

EXAMPLE: fcc Pb (lead)
from ESPRESSO/Wannier90, DFT-LDA



Given More Time, We Would...

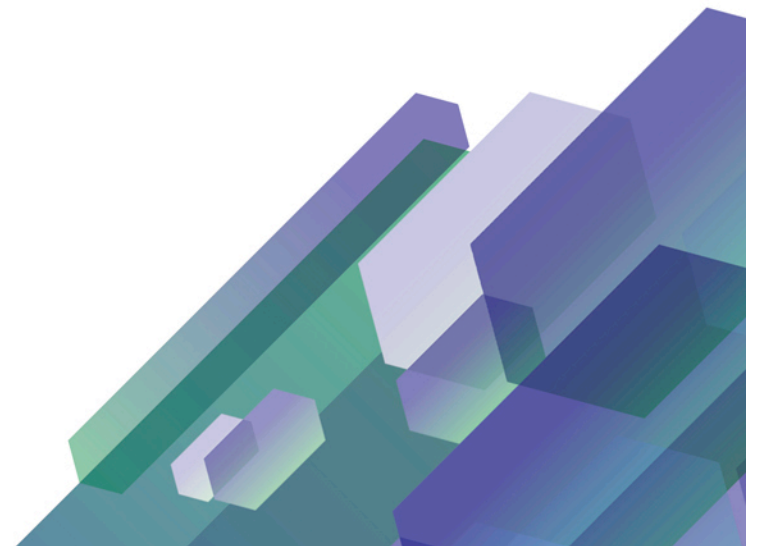
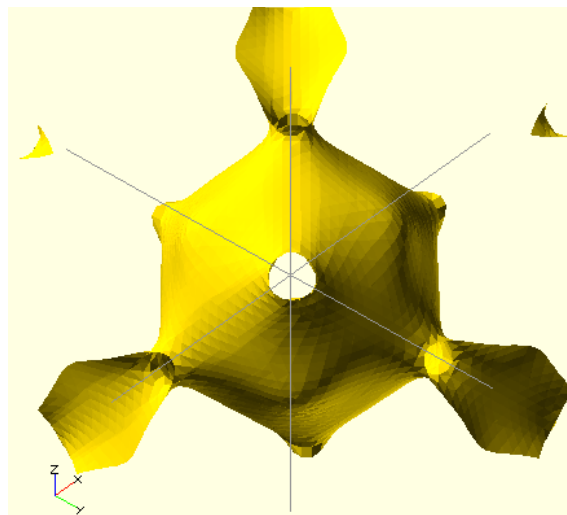
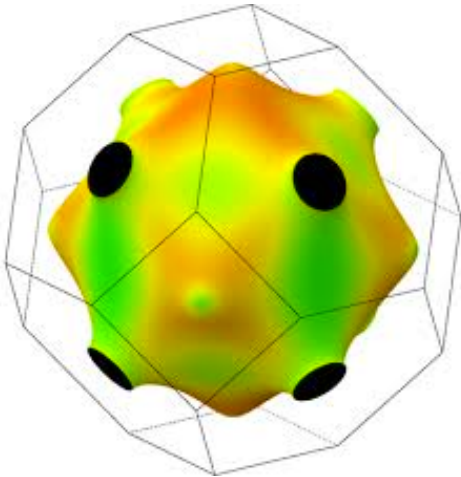


Support open-orbit Fermi surfaces better (e.g. Cu)

Better definition of first Brillouin zone

Improve user-interface

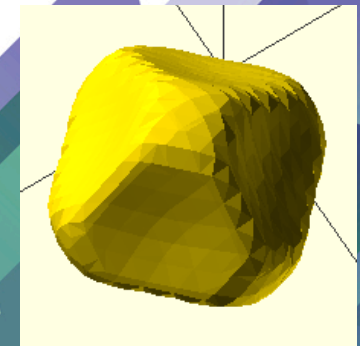
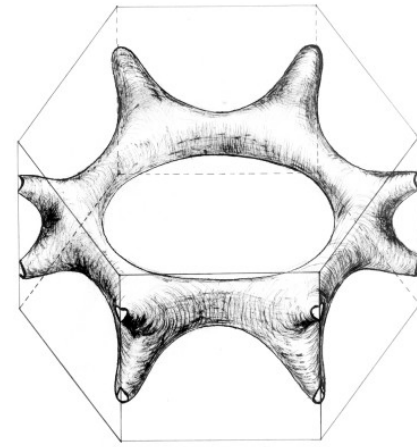
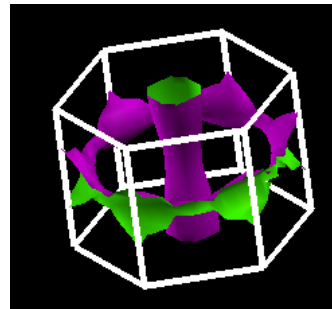
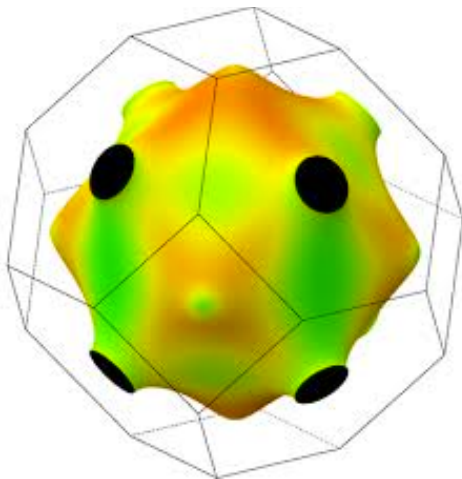
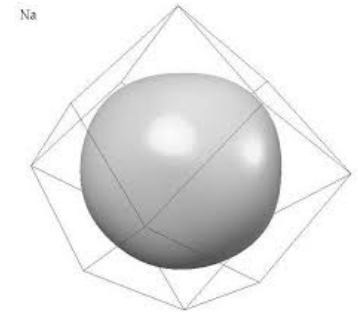
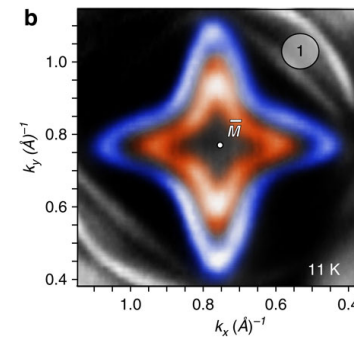
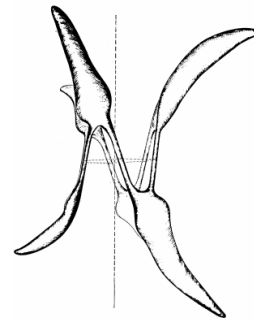
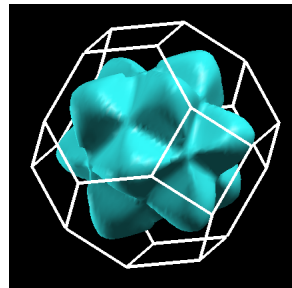
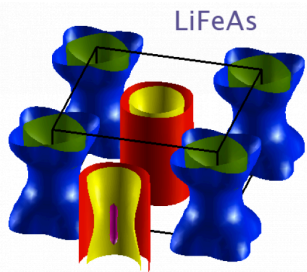
Offer more examples



Final One-Sentence Pitch!



Explore “Fermi-ology” from real calculations:
Visualize complicated and interesting 3D shapes
of Fermi surfaces for education and research!





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Q&A