

J-ICE: How to create nice 3D maps ? - 1

0. Generate cube with CRYSTAL (for instance)

ECH3

100

POT3

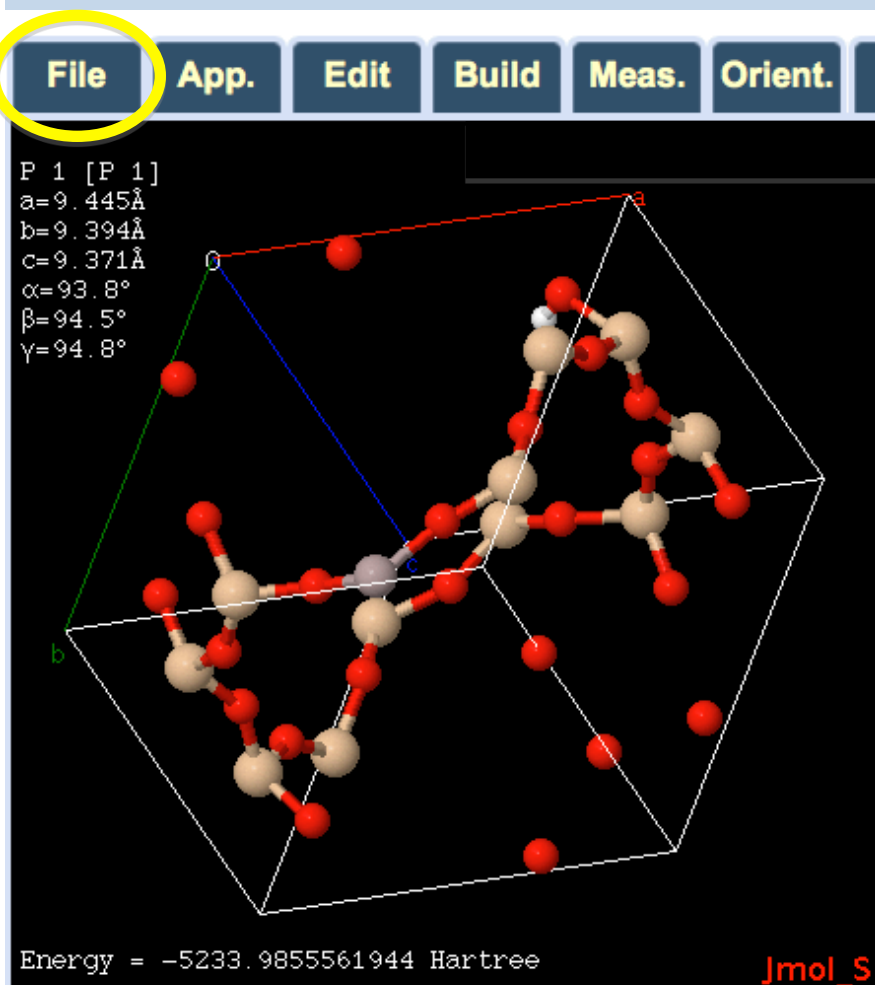
100

5

END

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1. Load the desired output



Primitive cell

File manager

Load File
Load New FILE

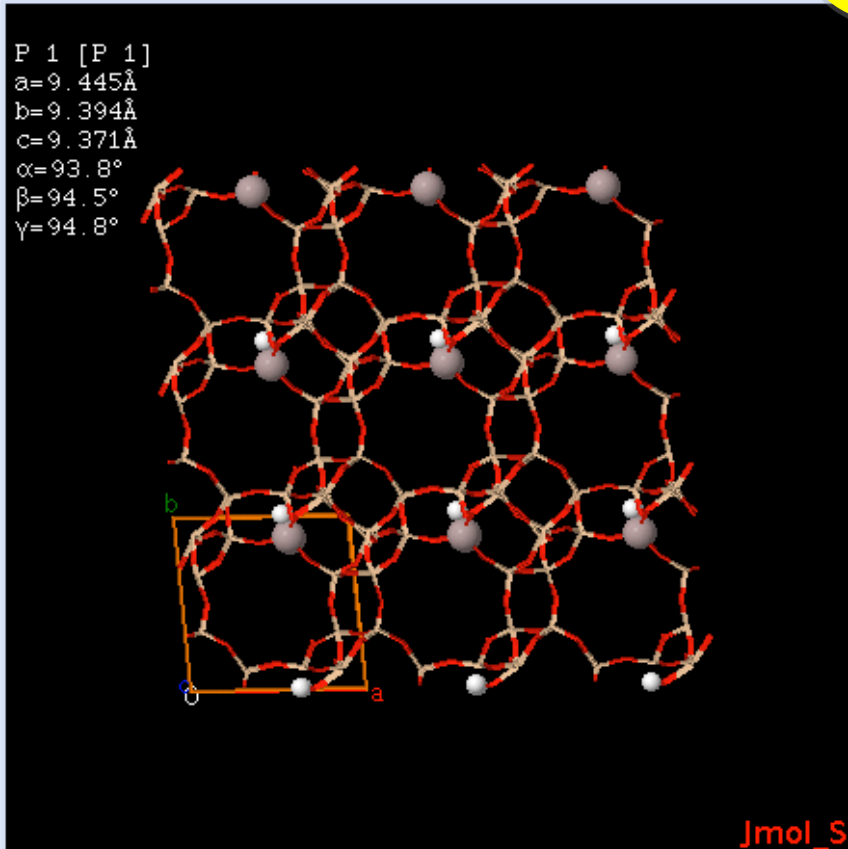
Filename

Export/Save File
Export File

J-ICE
release 1.0.5
by Pieremanuele Canepa
powered by Jmol
Please DO CITE:
"J-ICE: a new Jmol interface for handling and visualizing Crystallographic

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2. Expand the cell to get a piece of crystal



Cell properties

View Cell View axes

Cell style: size dotted dotted, color

Set cell: primitive conventional

Auto Pack Choose Pack Range

Supercell:

a: b: c: Å force supercell (P1)

Offset unitcell

Common sets

Manual set x: y: z:

Cell parameters (selected model)

Unit: Å Bohr

a b c

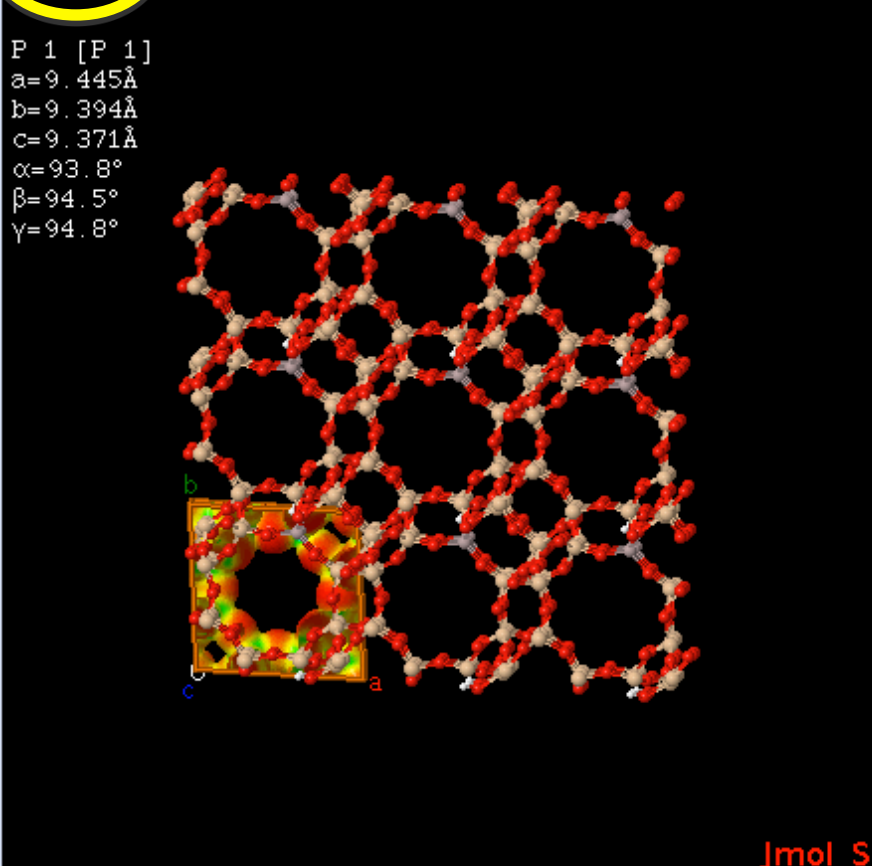
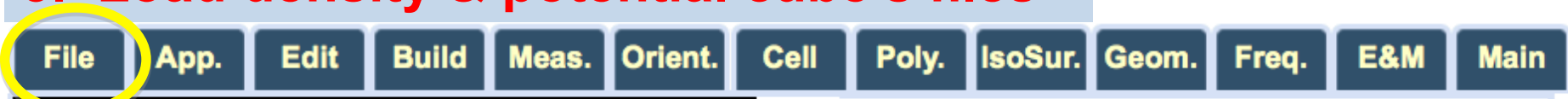
α β γ degrees

Volume cell Å³

3x3x3 packing

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3. Load density & potential cube's files



File manager

Load File

- Load New FILE
- Load New FILE
- Load generic (*.*)
- Load CIF (*.cif)
- Load XYZ (*.XYZ)
- Load CASTEP (*.cell)
- Load CRYSTAL (*.out)
- Load FHI-aims (*.in)
- Load GAUSSIAN0X (*.*)
- Load GROMACS (*.gro)
- Load GULP (*.gout)
- Load Material Studio (*.*)
- Load PDB (*.pdb)
- Load QuantumESPRESSO (*.out)
- Load ShelX (*.*)
- Load VASP (OUTCAR)
- Load VASP (*.xml)
- Load WIEN2k (*.out)
- Load map (*.CUBE)**
- Load map (*.jvxl)

Interface for Crystallographic and Electronic properties

"J-ICE: a new Jmol interface for handling and visualizing Crystallographic and Electronics properties.
P. Canepa, R.M. Hanson, P. Ugliengo, M. Alfredsson,
...

Follow **automatic procedure** once click on "Load map"

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4. NOW EXPAND THE WHOLE MAP

File App. Edit Build Meas. Orient. Cell Poly. **IsoSur.** Geom. Freq. E&M Main

Brønsted site

P 1 [P 1]
a=9.445Å
b=9.394Å
c=9.371Å
α=93.8°
β=94.5°
γ=94.8°

To survey the surface

Try different coloring & view options

IsoSurface

Classic isoSurfaces:
no isosurface remove iso

To adjust color range

-0.05714525 + 0.500000 a.u.

Colour-scheme Rainbow (default) Update map

Expand isoSurface periodically
a: 3 b: 3 c: 3 packIso

Style isoSurface:
 opaque translucent
 dots no-fill mesh

Color IsoSurface:
 Measure value

Show structure beneath Show cell