

Visualization Toolkit for Analyzing Defects in Materials

(a) Import Compound Data

(b) Import Defects Data

(c) Import DOS Data

Visualization Toolkit

(a) VTAnDeM Import Compound Data — □ ×

☐ Element ☒ Compound

Compound Name: ?

Data Directory:

Submit

/path/to/Cu2HgGeTe4

- CONTCAR
- OSZICAR
- OUTCAR
- POSCAR
- vasprun.xml

(b) VTAnDeM Import Defects Data — □ ×

Compound Name: ?

Data Directory:

Supercell Size, x:

Supercell Size, y:

Supercell Size, z:

Submit

/path/to/CHGT_Defects

- Cu_Hg
 - q-1
 - OSZICAR
 - OUTCAR
 - q+1
 - q0
- Hg_Cu
- V_Cu

(c) VTAnDeM Import DOS Data — □ ×

Compound Name: ?

DOSCAR File:

Submit