
 **Computational Materials Physics** 

Center for Molecular Modeling Department of Materials Science and Engineering

---

cif files, and how to find them

---

Stefaan.Cottenier@ugent.be <http://molmod.ugent.be>  
Technologiepark 903, Zwijnaarde <http://www.ugent.be/ea/dmse/en>  
my talks on Youtube: <http://goo.gl/P2b1Hs>

---

---

---

---

---

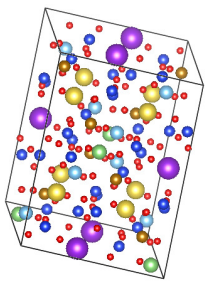
---

---

---

DFT input

physical input	technical input
----------------	-----------------



- XC-functional
- basis set size
- k-mesh
- ...

---

---

---

---

---

---

---

---

C  
rystallographic  
I  
nformation  
F  
ile

---

---

---

---

---

---

---

---

COD : [www.crystallography.net](http://www.crystallography.net)

ICSD : <https://icsd.fiz-karlsruhe.de>

MP : [www.materialsproject.org](http://www.materialsproject.org)

---

---

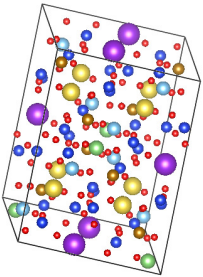
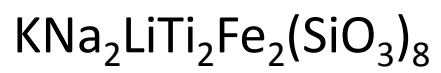
---

---

---

---

---



---

---

---

---

---

---

---