**Flourite and Anti-Flourite Structures**

Fluorite (AX2)

CaF2

CeO2

ZrO2

UO2

AntiFluorite (A2X)

**Mg2Si**

<http://www.amse.org.cn/fileup/PDF/E2010090.pdf>

Mg2Si has anti-fluorite structure under ambient conditions (space group Fm-3m). The silicon atom occupies the (0,0,0) site and the magnesium atoms occupy the (0.75, 0.25, 0.25) sites

<http://www.sciencedirect.com/science/article/pii/0038109871901323>

Mg2Si nanoparticle – Raman

<http://nanocon2012.tanger.cz/files/proceedings/14/reports/2228.pdf>

Be2C, Be2Si

Mg-2p63s2

Si-3s23p2

-bandgap 0.6-0.8eV

Li2O

Na2O

K2O

Point defect behavior in UO2 using approximation beyond DFT

Dorado (Journal of Physics: Condensed Matter) 2013

1. DFT + U and hybrid functionals for correlated electrons.
2. Circumvention of metastable states
   1. Occupation Matrix Control
   2. U-ramping
   3. Quasi-annealing