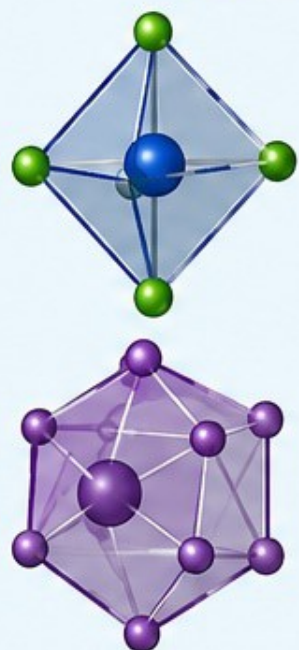


High-Pressure Behavior of MgAgF₃ Perovskite

0 GPa
Crystal
Structure

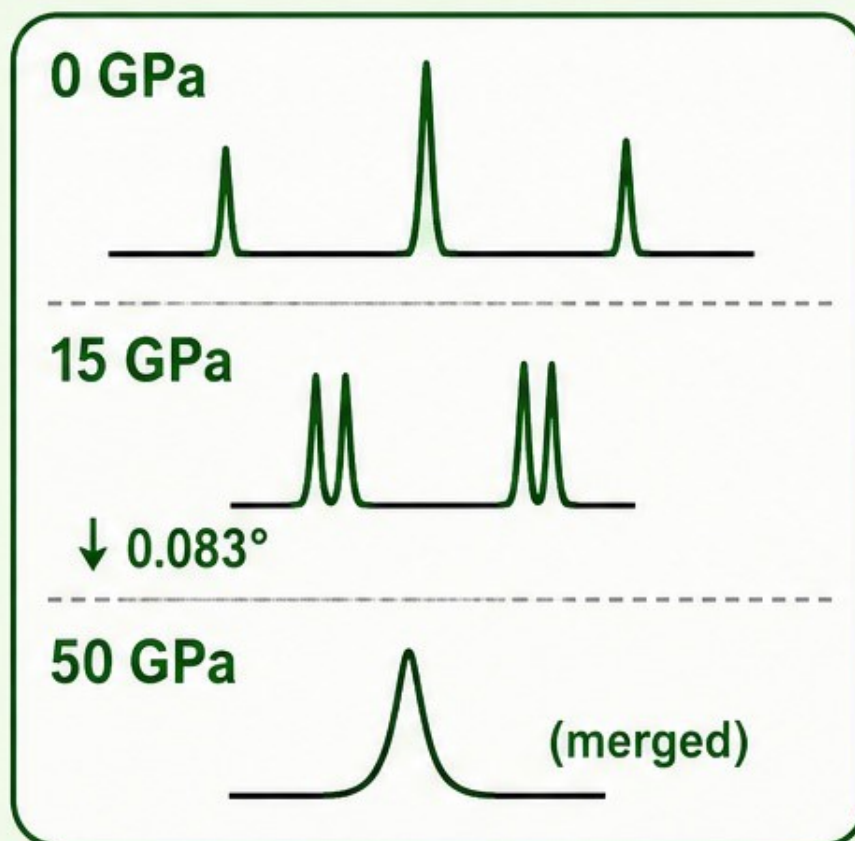


Mg
F₆

Ag
9-fold

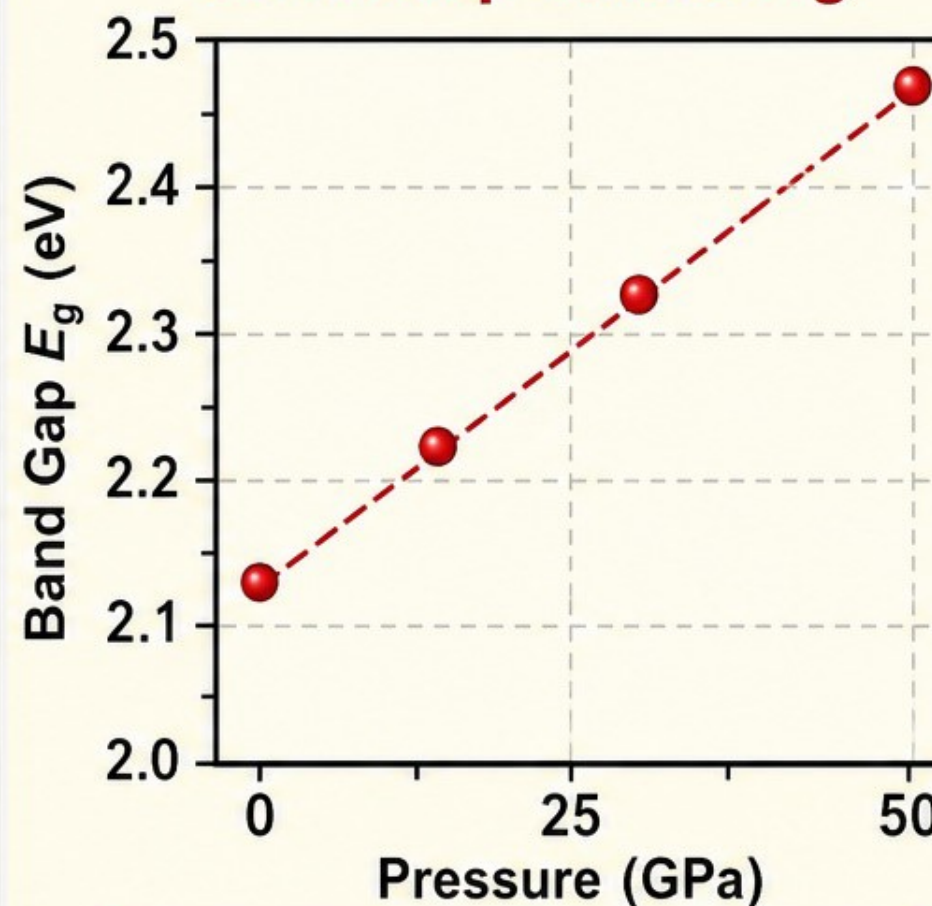
$a = 5.515 \text{ \AA}$
 $c = 13.549 \text{ \AA}$

XRD Evolution

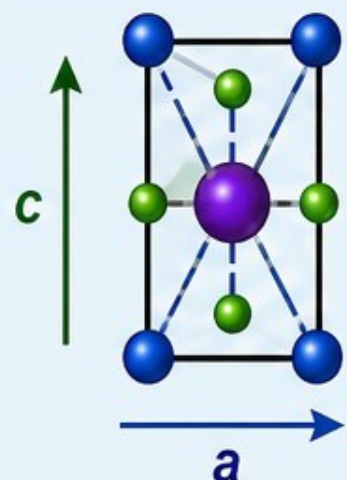


Simple → Doublet → Single

Band Gap Widening



$$E_g = 2.137 + 0.00667P$$

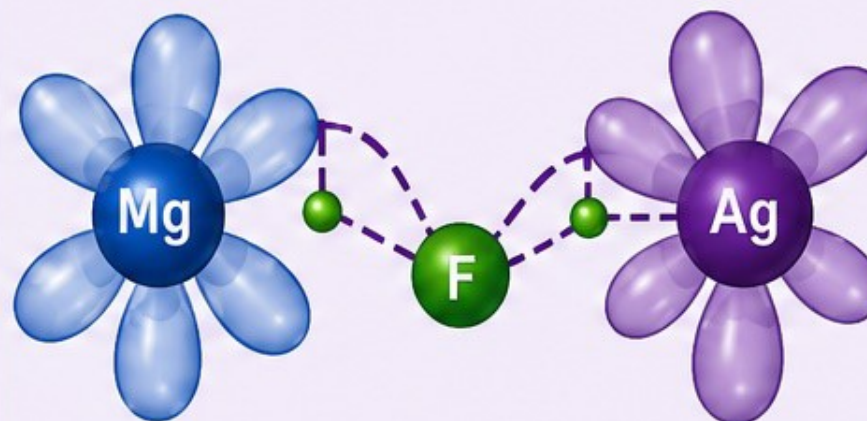


Anisotropic Compression:

$$B_{0,a} = 280.6 \text{ GPa} \quad B_{0,c} = 185.5 \text{ GPa}$$

Volume reduction:

22.2% at 50 GPa



Induced *d*-states
in Mg
(Pressure-induced
hybridization)