

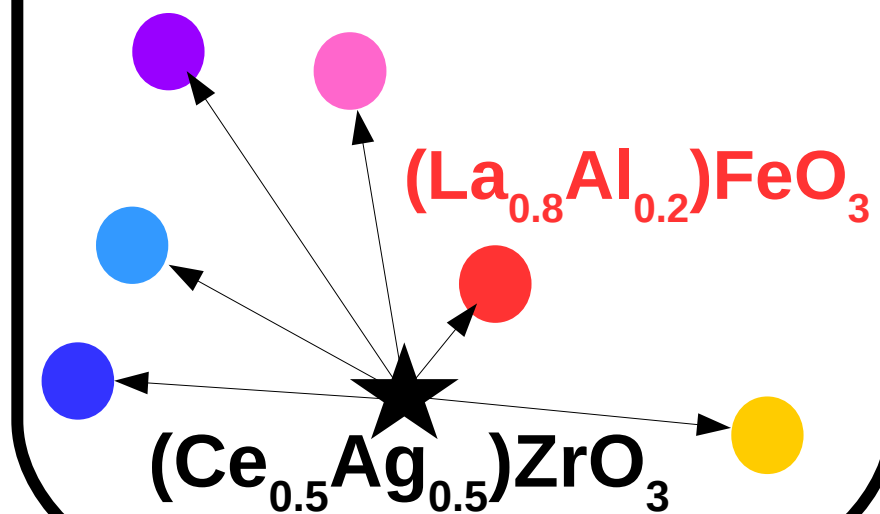
get experimental  
structure (cif)

replace atoms  
and fractions

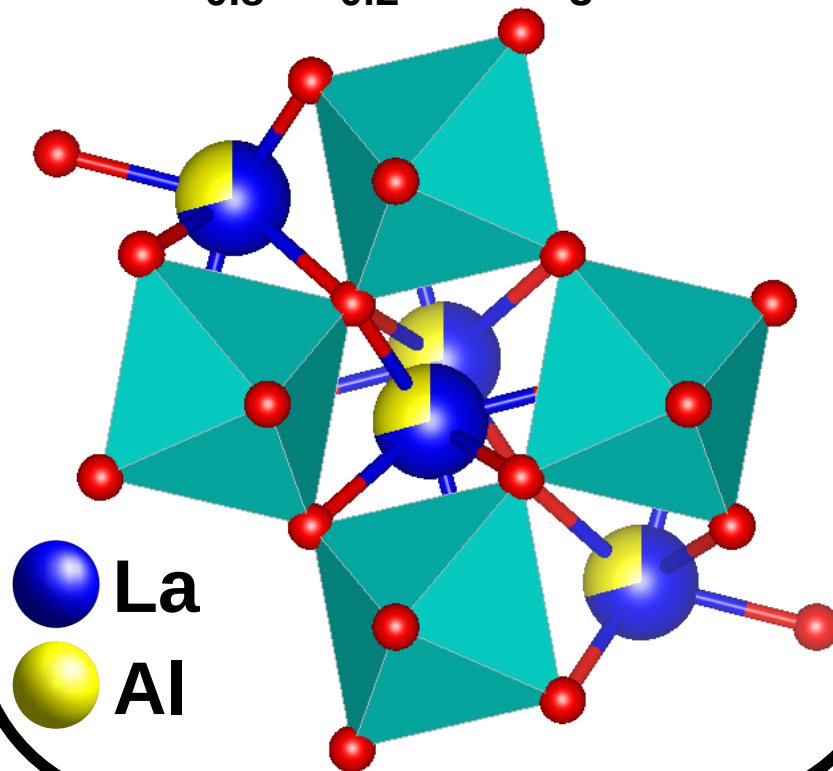
generate  
supercell

DFT geometry  
optimization

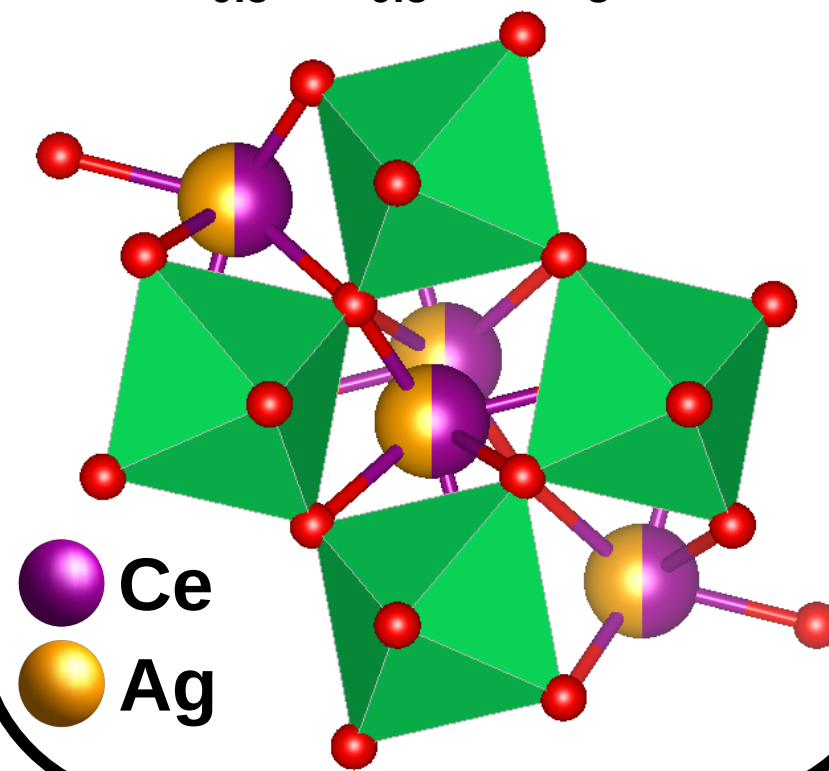
Find an analogous  
experimental  
composition



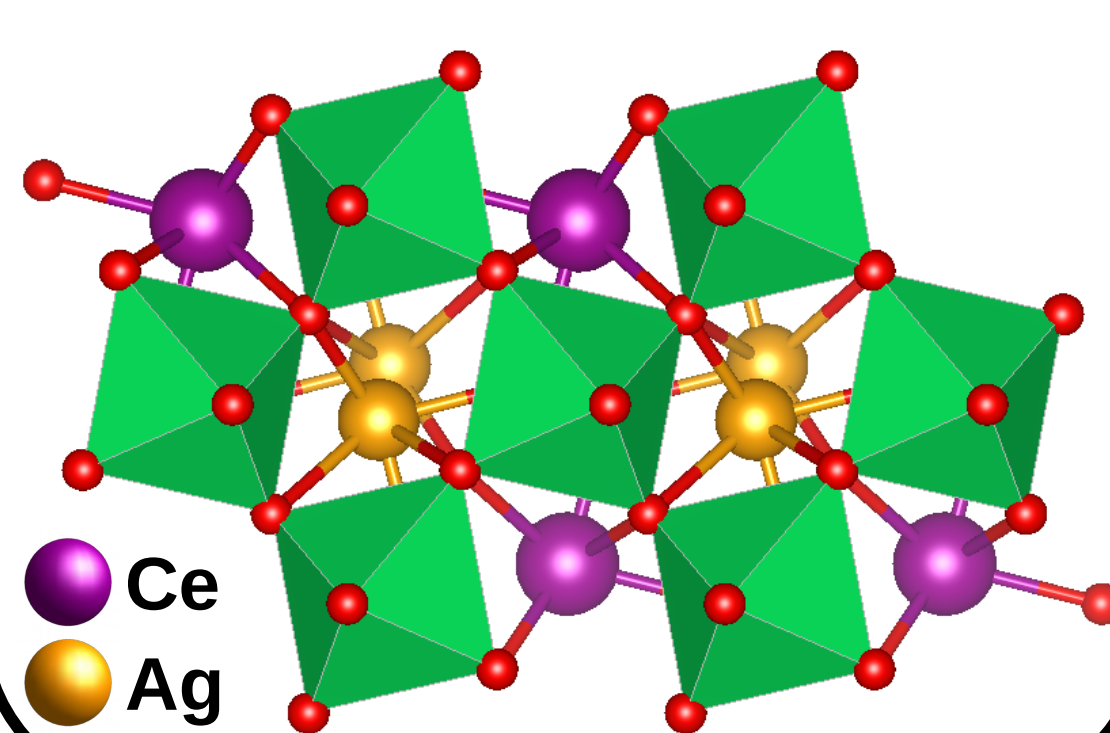
$(\text{La}_{0.8}\text{Al}_{0.2})\text{FeO}_3$  (.cif)



$(\text{Ce}_{0.5}\text{Ag}_{0.5})\text{ZrO}_3$  (.cif)



2x1x1 supercell



Optimized structure

