



**MATERIALS SCIENCE  
& ENGINEERING**  
TEXAS A&M UNIVERSITY

# Introduction to Materials Science & Engineering

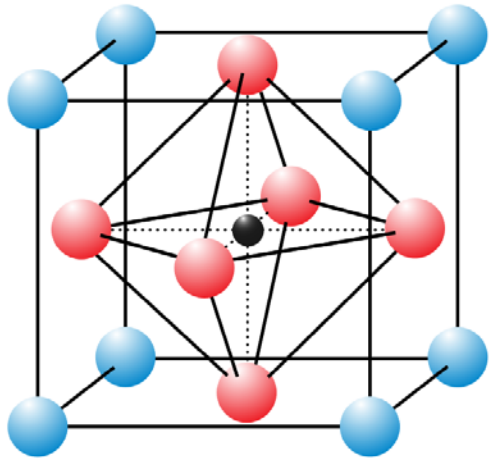
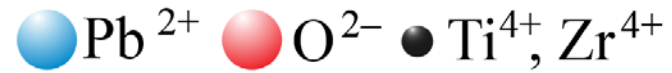
## Ionic Crystal Structures

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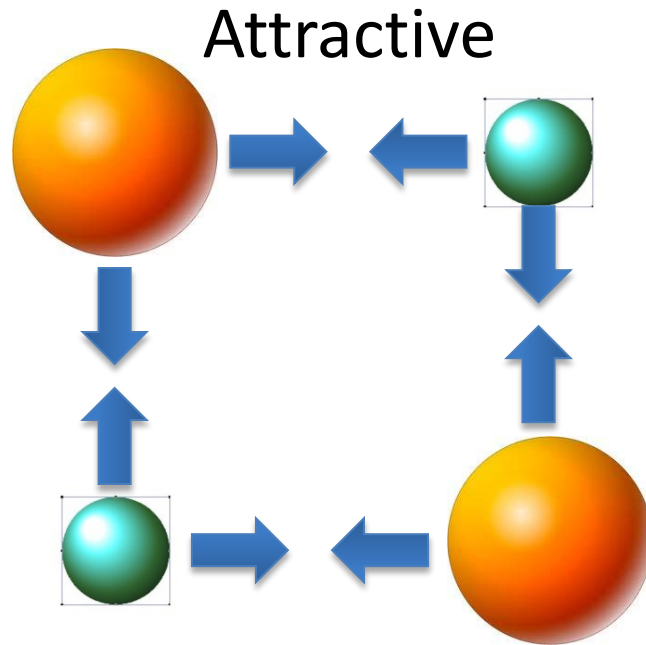
# Ionic Structures



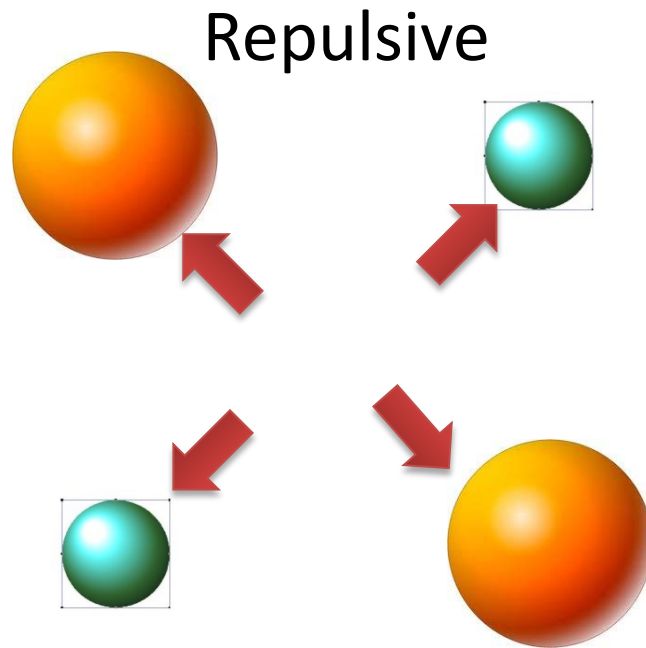
$$T > T_c$$

Wikipedia.org

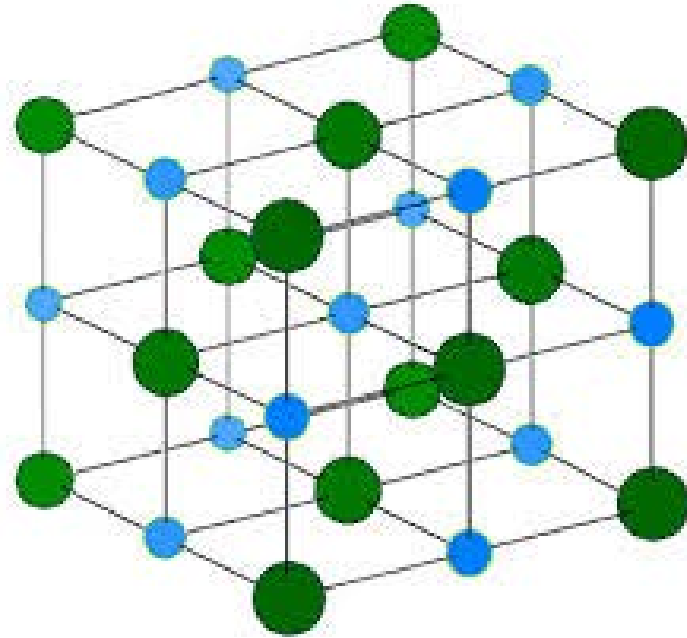
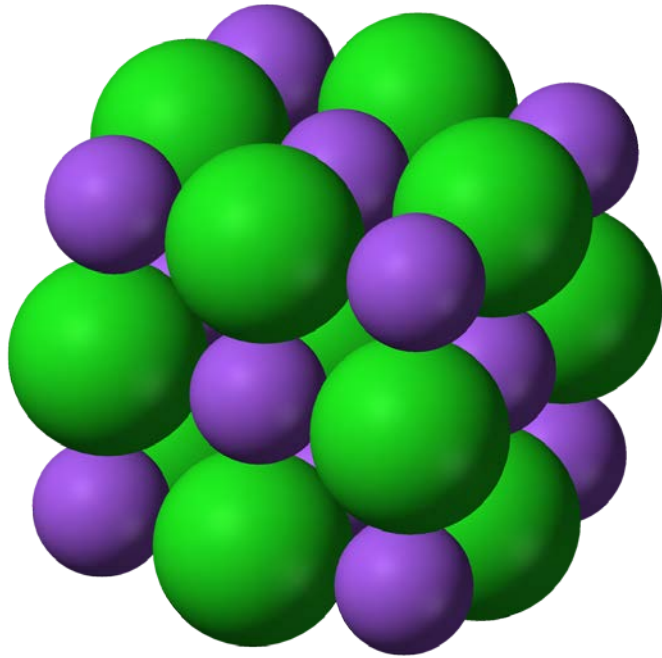
# Ionic Structures



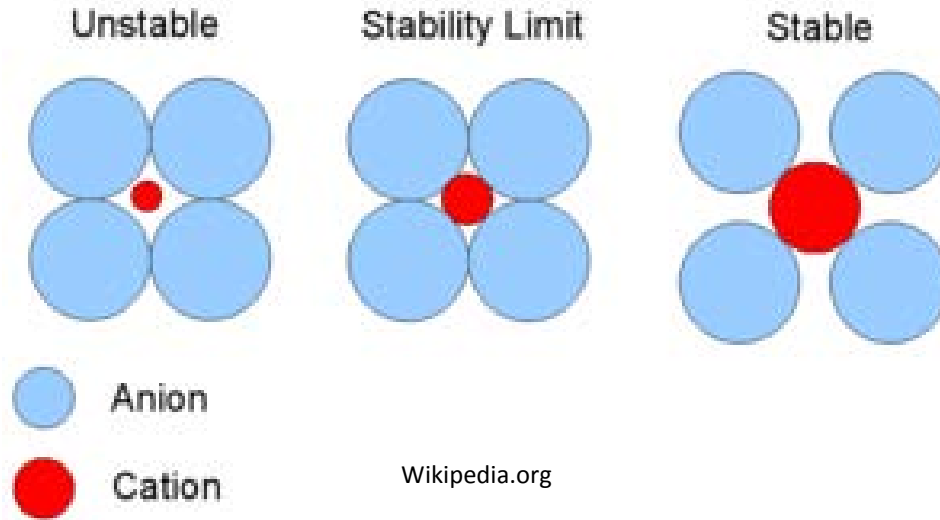
# Ionic Structures



NaCl

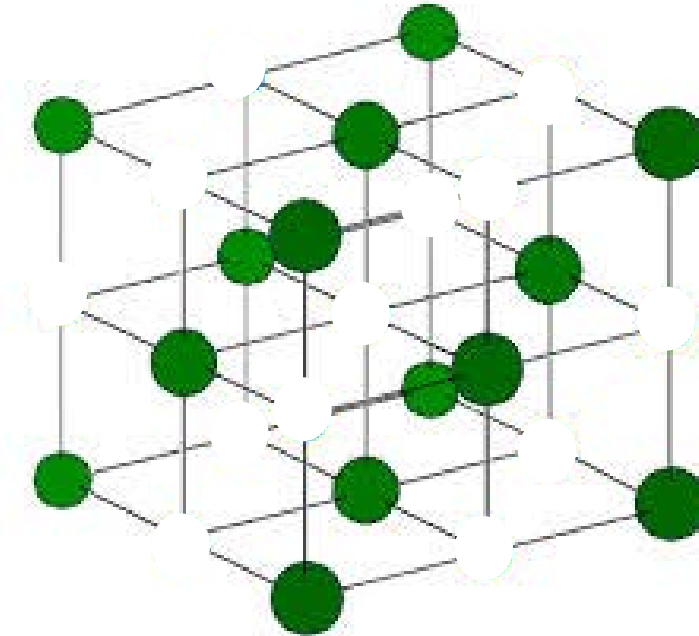
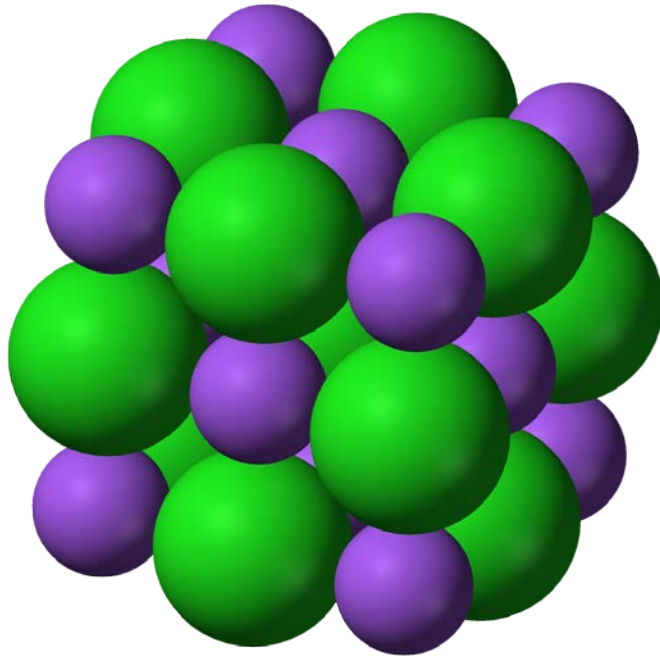


# NaCl: Which sites?



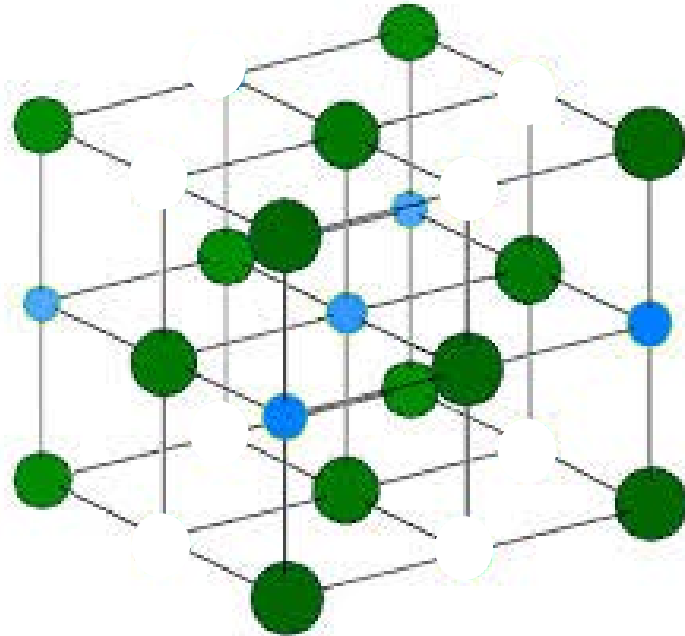
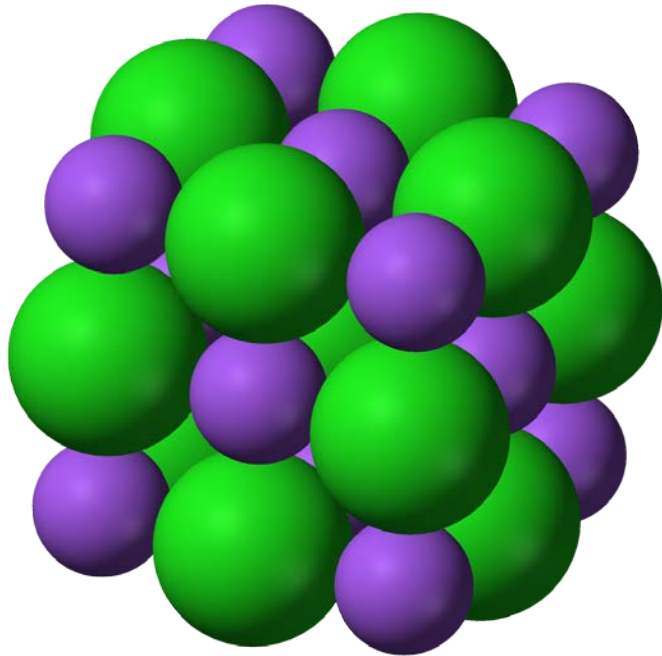
Rule: Cations will occupy the *largest* available site with  $r_{\text{site}} \leq r_{\text{cation}}$ .

# NaCl: Which Sites?



Radius Ratio	CN	Coordination
1.0	12	Cubic closest packed (CCP) Hexagonal closest packed (HCCP)
1.0–0.732	8	Cubic
0.732–0.414	6	Octahedral
0.414–0.225	4	Tetragonal
0.225–0.155	3	Triangular
<0.155	2	Linear

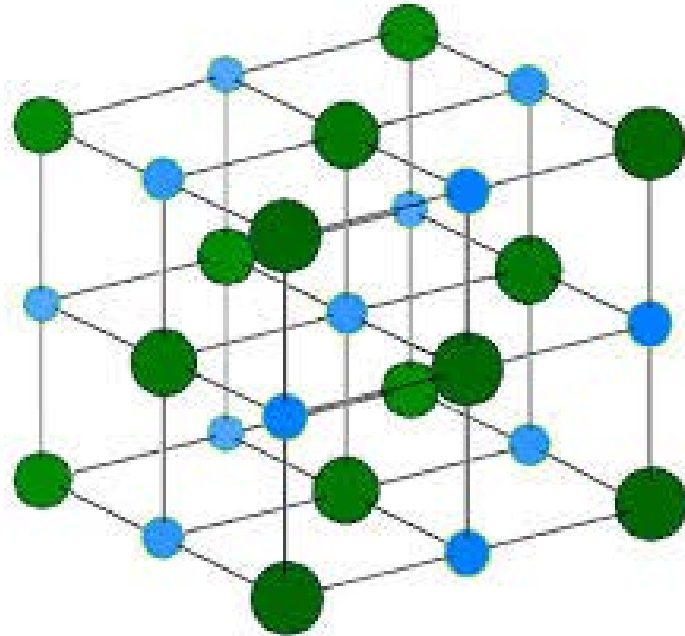
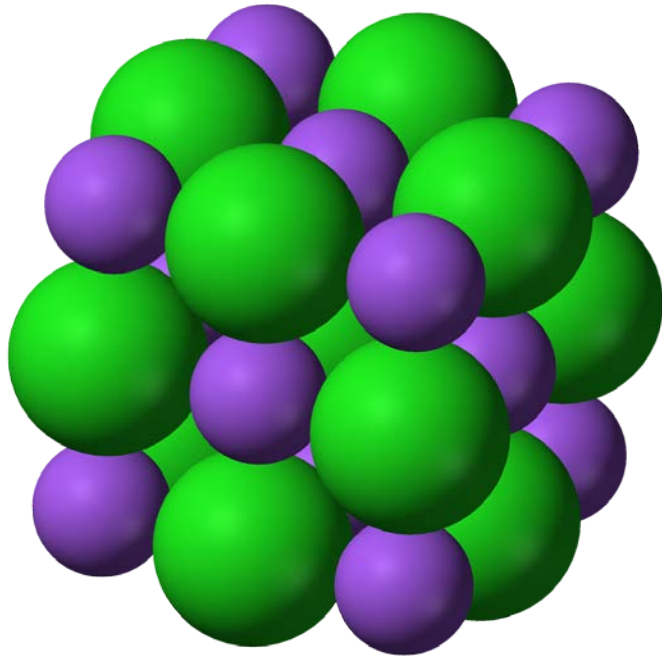
# NaCl: How Many Sites?



$\frac{1}{2}$  the octahedral sites occupied



# NaCl: How Many Sites?



ALL the octahedral sites occupied

# Summary

- Close-packed hard-sphere model
- Ionic radius ratio  $\rightarrow$  which sites
  - Certain lattices have or do NOT have certain sites
- Stoichiometry  $\rightarrow$  how many sites