

Survey of Materials

Homework 1, due date is set in Canvas LMS

Notes: In multiple choice problems explain your answer. Add references if needed. Upload solution as a single file "YourName.pdf" or "YourName.zip".

Scales

1. Maximum possible voltage of a metal-ion battery with a given cathode (we would like to optimize cathode) is primarily determined by material structure at: (A) atomistic scale (e.g. unit cell of the cathode crystal); (B) mesoscale (morphology of the cathode at nanometer to micrometer scales); (C) macroscale (device structure).

Composition-property relationships

2. You would like to create a catalyst, what elements are most important for this: (A) halides; (B) fluorine; (C) hydrogen; (D) transition metals; (E) rare-earth elements; (F) radioactive elements.

Material structural properties

3. Identify correct statement(s) about close-packed structures (not to be confused with ideal ball packing): (A) They can be defined as structures with high coordination number in the first coordination shell; (B) They can be defined as structures with high atomic packing factor; (C) Covalent solids never form close-packed structures; (D) Most of metals form close-packed structures; (E) Both anion and cation sublattices in most of binary ionic crystals are close-packed; (F) BCC lattice is close packed; (G) Diamond lattice is close-packed; (H) Point particles with isotropic binary interactions prefer close-packed structures.

Material electronic properties

4. By electrical conductivity we distinguish several classes of materials including: (A) metals, (B) semiconductors, (C) insulators, (D) superconductors, (E) solid ionic conductors, (F) electrolytes. Which of them do not define/constitute a separate class by electronic properties?

Bonding

5. Explain bonding in gallium crystal.

Basic geometry of molecules

6. For ethane molecule determine point group, asymmetric unit, and independent geometrical parameters (two sets: coordinates and internals).

Basic geometry of crystals

7. For graphite crystal determine space group, asymmetric unit, and independent geometrical parameters (two sets: coordinates and internals).

Crystallography

8. Calculate relative atomic packing factor and determine coordination number for Ga (http://zhugayevych.me/CryStr/Cryst/Ga_a.cif).

9. Given lattice coordinates of an atom in the rhombohedral setting, $(1/6, 1/3, 1/2)$, calculate the lattice coordinates of this atom in the hexagonal setting.

Total energy and thermodynamics of materials

10. The formation energies of possible binary compounds are: $E(A) = 1$, $E(B) = 2$, $E(AB) = 2.2$, $E(AB_2) = 2.3$, and $E(A_2B_3) = 2.4$ eV/atom. List compounds unstable with respect to phase separation.