

Survey of Materials

Homework 1, due date is set in Canvas LMS

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

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

2. You would like to create a material for solar cells for large scale electricity generation, what chemical elements would you consider: (A) lightweight; (B) radioactive; (C) abundant; (D) metals; (E) transition metals; (F) elements of main group IV; (G) compounds with covalent bonding; (H) compounds forming two-dimensional layers.

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.

4. What materials readily form amorphous structures rather than crystalline: (A) metals; (B) ionic solids; (C) covalent solids; (D) molecular solids; (E) polymers.

5. Explain bonding in gallium crystal.

6. List all independent geometrical parameters of adamantane molecule. What is the point group and fundamental domain (asymmetric unit) of this molecule?

7. List all independent geometrical parameters of graphite crystal. What is the space group and fundamental domain (asymmetric unit) of this crystals?

8. For anatase crystal determine the Wyckoff positions of voids and bonds. Determine Miller indexes for rectangles (not squares) formed by four nearest neighbor Ti atoms.

9. From the band structure shown here <http://zhugayevych.me/edu/Materials/images/bands.jpg>, determine bandgap(s) and bandwidth(s). Speculate on possible chemical composition and crystal structure.