Survey of Materials
Homework 2, 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. Which is not a principle of materials structure prediction: (A) close packing; (B) close copacking; (C) local coordination; (D) lowest energy; (E) Lewis octet rule; (F) Huckel's rule; (G) Hund's rules; (H) Hume–Rothery rules.

2. What is the lowest coordination shell at which B3 and B4 structural types are qualitatively different? What is the difference?

3. Calculate the relative atomic packing factor for In (http://zhugayevych.me/CryStr/Cryst/In.cif).

4. Fermi energy: (A) is the energy of the highest occupied one-electron orbital; (B) is the energy of the middle of the bandgap; (C) is the chemical potential; (D) applies only to fermions; (E) applies only to electronic systems without bandgap.

5. Estimate the energy of CH bond in the methane molecule, provided that the electronic energy of the molecule is -1467.066 eV, the electronic energy of the carbon atom is -1029.850 eV, and the CH distance is 1.093 Å.

6. Use CES EduPack Level 2 Sustainability database and Select Elements database. Answer the following questions (1 sentence per question): 1) What is "critical materials"; 2) What criteria are used to assess criticality; 3) Which elements are ranked as critical in the EU; 4) Why is Cerium on this list? 5) What steps can nations take to allay concern about critical materials?

7. Abrasives have high hardness. Make a bar-chart (CES EduPack, Level 3) of hardness and identify four materials with the highest values (Box selection option). They are of prime choice for abrasive wheels and pastes.

8. List at least three important material requirements for the conducting channel of a field effect transistor.

9. List at least three important power conversion losses in solar cells.

10. Show that the effective mass is proportional to the bandgap for the following tight-binding model of π-conjugated polymers: an infinite 1D chain of sites whose on-site energies alternate as $\pm\epsilon$ and nearest neighbor electron transfer integrals alternate as $t \pm \Delta t$.