

Survey of Materials

Homework 2, 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".

Electronic structure

1. From the band structure shown here <http://zhugayevych.me/edu/Materials/images/bands.png>, determine bandgap(s) and bandwidth(s). Speculate on possible chemical composition and crystal structure.
2. Does the figure <http://zhugayevych.me/edu/Materials/images/bands2.png> show electron or phonon dispersion? What information about material can be inferred from it?
3. Identify/interpret occupied localized molecular orbitals in <http://zhugayevych.me/edu/Materials/images/LM0.mgf> (DFT calculations), that is determine core/bonding/non-bonding/LP orbitals, $\sigma/\pi/\delta$ bonding, AO composition.

Semiconductors

4. Which structural types are hardly possible for semiconductors: (A) A1; (B) B1; (C) C1; (D) E1₁; (E) E2₁; (F) A4; (G) B4; (H) C4.
5. List at least three important power conversion losses in solar cells.

Structural materials

For this topic see separate assignment in Canvas (graded separately).