

## Survey of Materials

### Homework 3, 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. Explain why among alkali metals (Li, Na, K, Rb) Li has the lowest standard electrode potential ( $-3.04$  V), despite its highest ionization potential ( $+5.4$  eV) and highest cohesive energy?
2. Calculate and compare theoretical specific capacity for  $\text{LiCoO}_2$ ,  $\text{Li}_2\text{CoPO}_4\text{F}$ , and  $\text{Na}_2\text{CoPO}_4\text{F}$ .
3. Why the catalytic activity for oxygen reduction reaction of perovskite oxides correlates with the orbital filling of  $e_g$  orbital of surface transition metal atoms? At what filling the largest catalytic activity is observed. *Hint:* [http://zhugayevych.me/edu/Materials/res/Rev\\_Suntivich11.pdf](http://zhugayevych.me/edu/Materials/res/Rev_Suntivich11.pdf).
4. Which of the following organic materials would exhibit effective electron injection from calcium electrode: (A) PCBM=phenyl-C61-butyric acid methyl ester; (B) rubrene; (C) polypropylene; (D) P3HT=poly(3-hexylthiophene); (E) PEEK(polyether ether ketone)-CNT(carbon nanotube) composite; (F) MEH-PPV=poly(p-phenylene vinylene) derivative? For materials data you can use e.g. Sigma-Aldrich product catalog.
5. Which molecule will be more effective for visible light absorption: (A) molecule with  $\sigma$ -frontier orbitals; (B) molecule with  $\pi$ -frontier orbitals; (C)  $\pi$ -conjugated molecule; (D) molecule with high splitting between HOMO and LUMO.
6. Assume you need to prepare a CNT-reinforced composite filament for your FDM 3D-printer. FDM process requires to use polyethylene matrix. Can you suggest possible operations with your CNTs at atomic level to increase your ultimate composite toughness?
7. Why do mechanical stresses arise in a solid?
8. Compare Young's modulus for structural materials: metals, ceramics, concrete, rubber, wood, fiber-reinforced composites.
9. For estimation of mechanical stresses, when analytical methods of calculation can be applied, and when only finite element analysis?