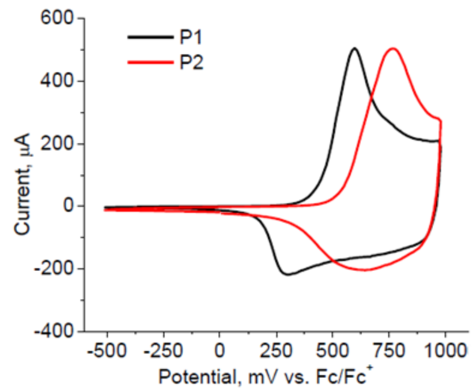
Organic Materials for Energy and Optoelectronics
Homework 2, due date is set in Canvas LMS
Topic: methods and applications

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

1. Which materials are not π-conjugated: (A) graphene; (B) graphite; (C) diamond; (D) polyyne; (E) polyacetylene; (F) polyethylene; (G) metal-organic frameworks; (H) transition metal dichalcogenides.

2. Below the cyclic voltammograms are presented for two different organic polymers, P1 and P2. What is the correct relation between HOMO and LUMO energy levels of P1 and P2 (do not forget that such values are negative):
(A) $E_{\mathrm{HOMO}}(\mathrm{P1}) < E_{\mathrm{HOMO}}(\mathrm{P2})$, $E_{\mathrm{LUMO}}(\mathrm{P1}) < E_{\mathrm{LUMO}}(\mathrm{P2})$;
(B) $E_{\mathrm{HOMO}}(\mathrm{P1}) > E_{\mathrm{HOMO}}(\mathrm{P2})$, $E_{\mathrm{LUMO}}(\mathrm{P1}) > E_{\mathrm{LUMO}}(\mathrm{P2})$;
(C) $E_{\mathrm{HOMO}}(\mathrm{P1}) < E_{\mathrm{HOMO}}(\mathrm{P2})$, $E_{\mathrm{LUMO}}(\mathrm{P1}) > E_{\mathrm{LUMO}}(\mathrm{P2})$;
(D) $E_{\mathrm{HOMO}}(\mathrm{P1}) > E_{\mathrm{HOMO}}(\mathrm{P2})$, $E_{\mathrm{LUMO}}(\mathrm{P1}) < E_{\mathrm{LUMO}}(\mathrm{P2})$.

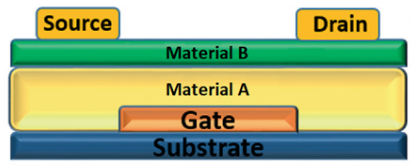


3. For an amorphous (e.g. thin film) conjugated polymer list all properties which is hard to simulate from first principles even approximately: (A) intramolecular structure such as bond lengths and angles; (B) morphology, i.e. material structure on scales up to its homogeneity; (C) UV-Vis spectra; (D) Raman spectra; (E) XPS; (F) NMR; (G) HOMO/LUMO energy levels; (H) charge carrier mobility.

4. List three most successful or potentially successful applications or classes of applications of organic semiconductors (excluding graphene).

5. Some organic semiconductors show better charge transport in amorphous phase rather than in crystalline. Speculate on possible origin(s) of such counterintuitive behavior.

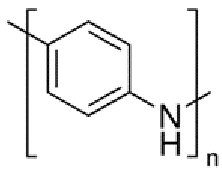
6. Determine possible composition of Materials A and B in the OFET device architecture shown in the figure (gate, source and drain are metal electrodes): (A) Material A=P3HT (poly(3-hexylthiophene)), Material B=PC60BM; (B) A=Al2O3, B=PVA (polyvinyl alcohol); (C) A=Al2O3, B=C60; (D) A=P3HT, B=PVA.

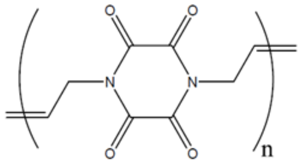


7. List materials requirements for electronic donor in bulk-heterojunction solar cells.

8. A laboratory-made organic solar cell with working area of 1.65 cm^2 is tested using solar light simulator with integral power $P_{\text{in}} = 100$ mW/cm^2. According to the I-V data, $V_{\text{OC}} = 0.95$ V, $J_{\text{SC}} = 26.6$ mA, and the maximum power of the working solar cell is achieved at 0.57 V and 24.1 mA. Calculate fill factor and power conversion efficiency.

9. Polyaniline (1) and poly-N,N'-diallyl-2,3,5,6-tetraketopiperazine (2) are redox active organic polymers used in organic electrodes for metal-ion batteries. For each compound, estimate maximum number of electrons per repeating unit it can reversibly take during charge/discharge and calculate the corresponding theoretical capacity in mAh/g.

(1) 

(2) 

10. Read a review article or watch a video mentioned in the last class ("Other applications"). Then in about five sentences describe a single application of organic semiconductors discussing importance of this application, suitable classes of organic materials, challenges, current progress, perspectives etc. Applications discussed in separate lectures (OFET, solar cells, batteries) cannot be discussed here.