

Organic Materials for Energy and Optoelectronics

Lab 1, due date is set in Canvas LMS

Topic: Modeling of organic semiconductors

Notes: Upload solution as a single file "YourName.zip". Provide absolute minimum of supporting info – no copies of work folders. Compare results with published data. Solution must be submitted as article-style report supplemented by data files if needed. Be prepared to give a 5 min presentation of everything that you consider nontrivial in your work.

Take a one-parameter series of molecules or polymers or crystals, and study dependence of their properties on the parameter. The parameter is usually a group of atoms which are modified across the series. You can take either your own data set or choose one of the proposed sets. If you are student of Computational Materials Science track you should perform all calculations by yourself, otherwise you can take available raw calculations in the form of unprocessed program output files. Below you will the list of proposed data sets and problem formulations.

- **Functionalized distyrylbenzene** [Lab1_OPV3OMe2.zip]: study dependence of HOMO/LUMO and excitation energies on the functional group.
- Any problem formulation similar to sample solutions listed below.

Sample solution: See Lab1_Klimovich21.zip