

README

Data underlying publication "Electron affinity and binding energy of excitons in disordered organic semiconductors. II. First principles simulations and inverse photoemission studies for MADN (Physical Review B, 2025).

The database contains Mathematica notebook files (.nb) and Excel files (.xlsx) that provide simulation and measurement data that are shown in the main paper and in the Supplemental Material.

Mathematica notebooks

The data are given in the form of lists. The specific curves to which each list refers is explained in the notebook files.

Excel files

- Figure-2(a-b)-041125.xlsx gives as a function of the depth z (nm) the vacuum average energy and its standard deviation (STD) (green data points), the static average energy and its standard deviation (STD) (blue data points), and the polar average energy and its standard deviation (STD) (red data points).
- Figure-6(a-b)-041125.xlsx gives as a function of the energy $E - \varepsilon_{vac}$ (eV) the contributions to the LEIPS spectrum from the LUMO, LUMO+1 ... LUMO+5 states (arbitrary units), the sum of these contributions and the instrumentally broadened total spectrum.
- Figure-7-LEIPS-spectra-051125.xlsx gives as a function of the energy E with respect to the vacuum energy ε_{vac} (eV) the measured LEIPS spectrum (units: counts per second), obtained for various bandpassfilter wavelengths (nm) and for various film thicknesses (nm). The two tabs gives data for alpha-MADN and beta-MADN.
- Figure-8(a-b)-041125.xlsx gives as a function of the depth z (nm) the difference between the ionization energy and the electron affinity and its standard deviation (adiabatic HOMO-LUMO gaps, green triangles), the S1 exciton energy $E_{0-0,A}$ and its standard deviation (blue squares), and the resulting exciton binding energy and its standard deviation (red circles).
- Figure-9a-alpha-MADN-061125.xlsx and Figure-9B-beta-MADN-061125.xlsx give as a function of the energy (eV) the theoretical optical absorption spectra for thin films of (a) α -MADN and (b) β -MADN (full blue curves).
The experimental curves in Figure 9 have been taken from E. J. de Jong, N. G. de Rooij, W. F. M. van Geel, C. Hauenstein, H. Tomita, G. Trimbo, M. Berghuis, S. Fukushima, S. Gottardi, B. Baumeier, H. Yoshida, and R. Coehoorn, Electron affinity and binding energy of excitons in disordered organic semiconductors. III. Multimethod study for films of the blue fluorescent emitter MADN (accepted), (2025, DOI: <https://doi.org/10.1103/kcl9-54vq>, data available from DOI 10.4121/d320a48b-aed4-49c3-9885-82cbac8ffe5d).
- Figure-10(abc)-041125.xlsx (Figure-10(def)-041125.xlsx) give for 393 (392) molecules the difference between the HOMO energy, LUMO energy, gap energy, S1 energy and exciton binding energy with respect to the mean value that has been used to in Fig. 10(a-c) and Fig. 10(d-f).
- Figure-S2-alpha-MADN-041125.xlsx and Figure-S2-beta-MADN-041125.xlsx give as a function of the energy the cumulative contribution to the relative permittivity due to vibrational modes.