**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) that provide simulation and measurement data that are shown in figures 3 and 4 of the main paper and in figures S3-S7 of 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.