Predicted energy-structure-function maps for the evaluation of small molecule organic semiconductors

Electronic Supplementary Information

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Supplementary information includes CIFs (Crystallographic Information File) of the predicted crystal structures of all molecules studies (molecule.cif), along with data files summarizing calculated information on each structure (molecule_data.txt):

pentacene_CSP.cif, pentacene_data.txt

TT_CSP.cif, TT_data.txt

5A_CSP.cif, 5A_data.txt

5B_CSP.cif, 5B_data.txt

5C_CSP.cif, 5C_data.txt

7A_CSP.cif, 7A_data.txt

7B_CSP.cif, 7B_data.txt

7C_CSP.cif, 7C_data.txt

The CIF files contain the calculated lattice energy (in kJ/mol) of each structure in the _data field.

The data.txt files contain one line per structure, ordered in increasing energy. The four columns are: lattice energy (kJ/mol); density (g/cm^3); structure classification (free text); charge mobility (cm^2/Vs). The charge mobility corresponds to hole mobility for pentacene and electron mobility for the azapentacenes. Charge mobilities are only calculated for structures up to 7 kJ/mol above the lowest energy structure (the global minimum).

7N Crystal structure landscapes

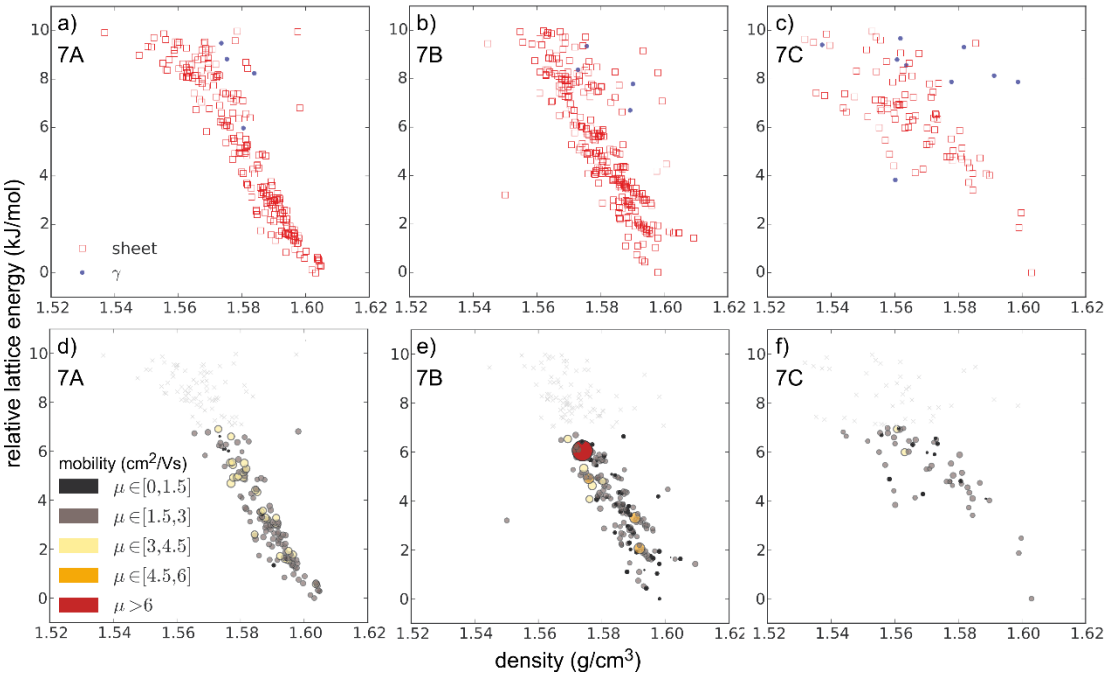

Figure S1. Predicted crystal structure landscapes for the 7N azapentacenes (a,d) **7A**, (b,e) **7B** and (c,f) **7C**. Each point corresponds to a distinct crystal structure. Plots on the left are categorised by crystal packing type. Colouring and the size of circles on the right-hand-side correspond to the magnitudes of calculated electron mobilities (in cm^2/Vs. Legends are shown in (a) and (d).

Weighting for average mobility calculations

The fitting of β for the weighted average mobility (equation 5 in main text) was to the distribution of polymorph lattice energy differences calculated by Nyman and Day (*CrystEngComm*, 17, 5154-5165 (2015)). We assume that the global lattice energy minimum in any CSP set is an observable polymorph. Therefore, the distribution of lattice energy differences between known polymorphs tells us the probability that any higher energy structure on the CSP landscape will be observed. The distribution of polymorph lattice energy differences fits an exponential decay; the fitting is shown in Figure S2. From this, we take β for equation 5 as 2.969 kJ/mol.

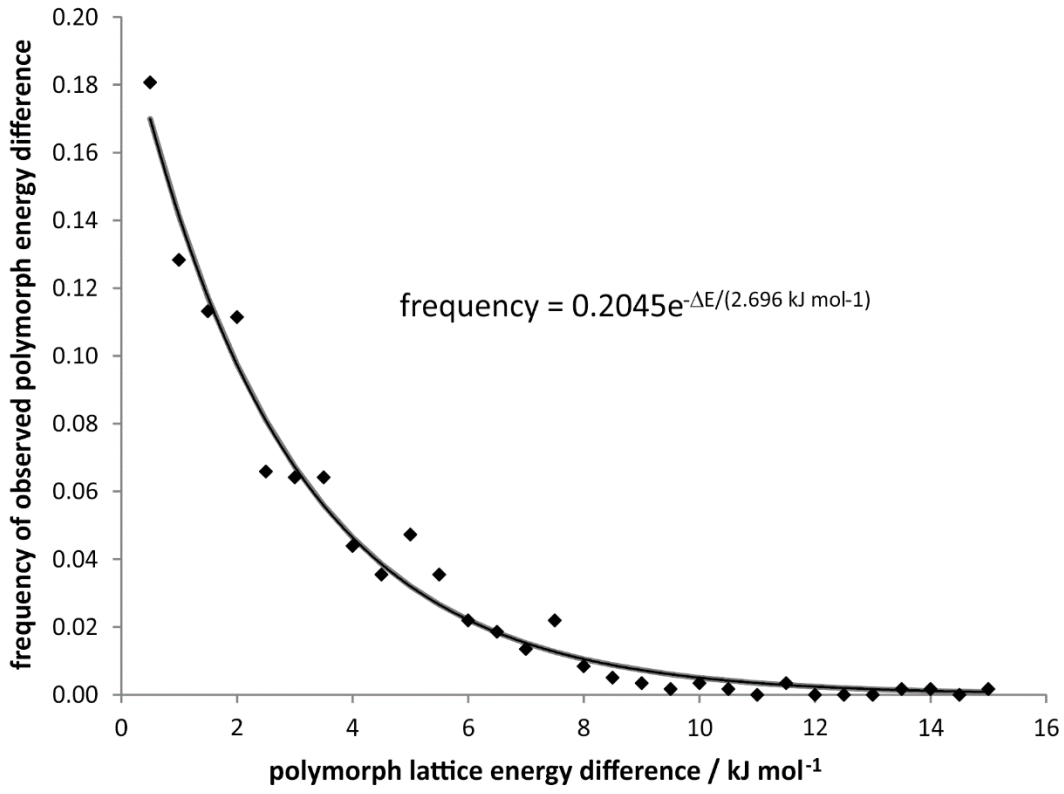

Figure S2. Exponential fit to the frequency of lattice energy differences between pairs of known polymorphs of organic molecules.