## **Supplementary information**

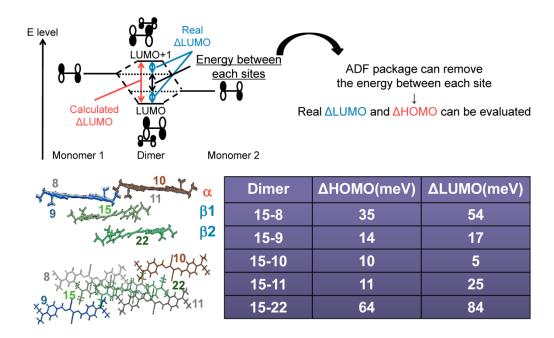


Figure S1

Summary of the HOMO/LUMO splittings calculated in different DE2 dimers using the ADF package.

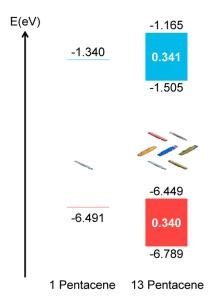


Figure S2

HOMO and LUMO splittings calculated for a 3D cluster of 13 molecules in pentacene crystal.