

Electronic Supporting Information

**Mapping the Configuration Dependence of
Electronic Coupling in Organic Semiconductors**

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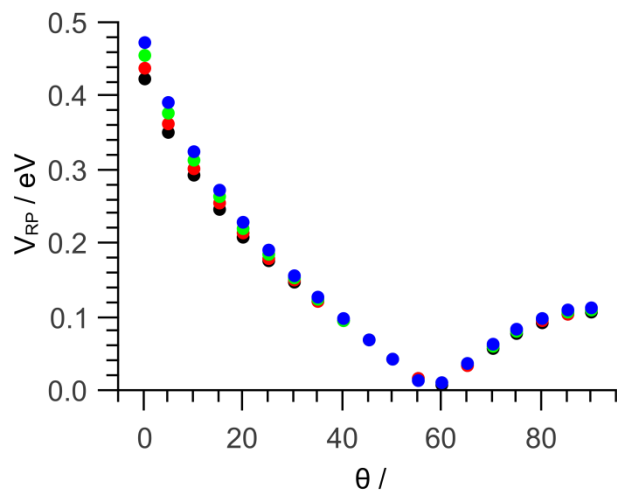


Figure S1. Comparison of V_{RP} for different acene lengths as a function of rotation angle theta. Naphthalene (blue), anthracene (green), tetracene (red) and pentacene (black).

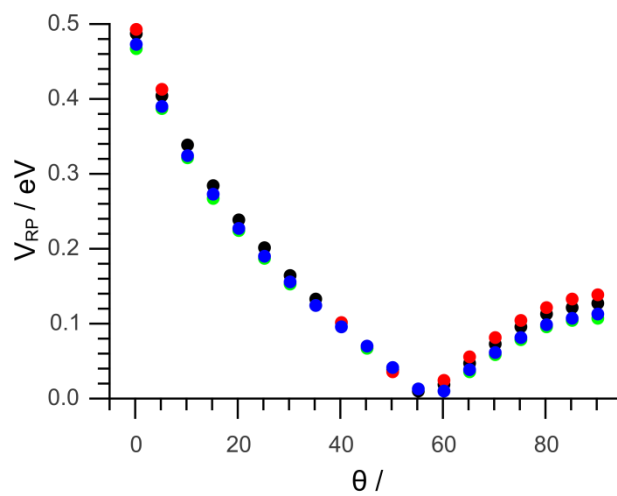


Figure S2. Effect of basis set on V_{RP} for a pair of naphthalene molecules with varying rotation angle theta. 6-31G (blue), 6-31G(d) (green), 6-31+G(d) (red) and 6-311G (black).

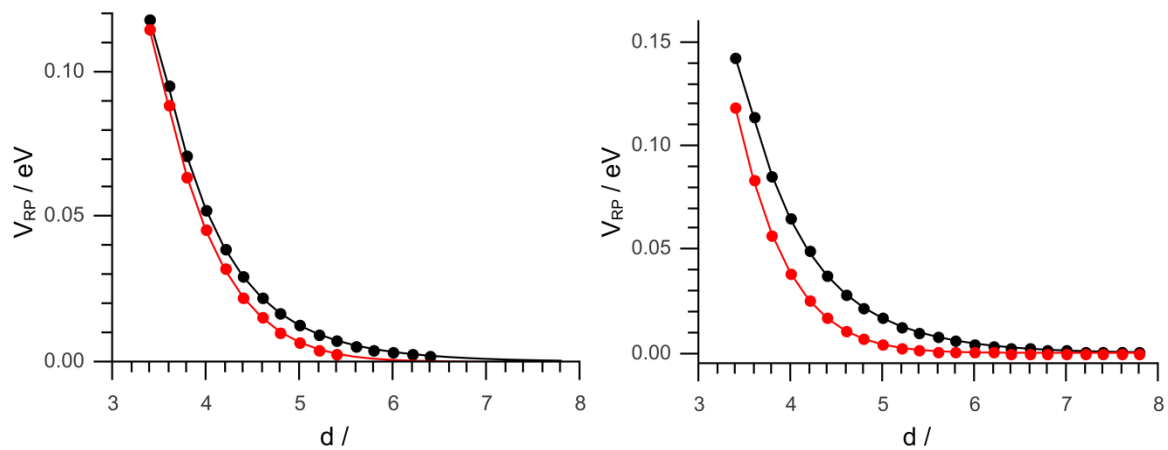


Figure S3. Effect of the basis set on V_{RP} for a naphthalene pair at a fixed rotation angle (40° (left) and 80° (right)) with increasing intermolecular distance.

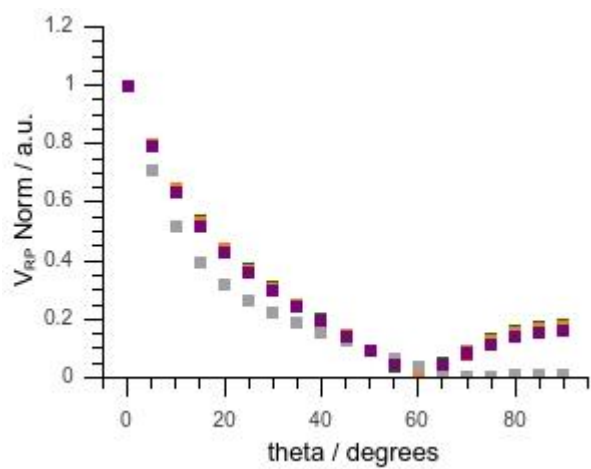


Figure S4. Normalized evolution of V_{RP} with molecular rotation for a naphthalene dimer with different functionals.

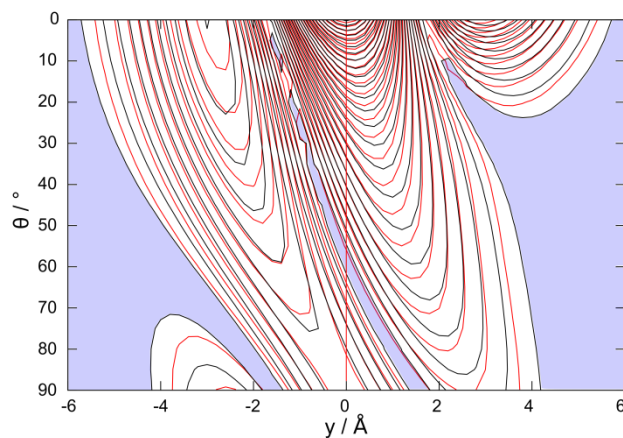


Figure S5. Comparison of V_{RP} (black, 0.02 eV) and S_{RP} (red, 0.005 a.u.) contours during molecular rotation and short axis displacement in a naphthalene dimer.

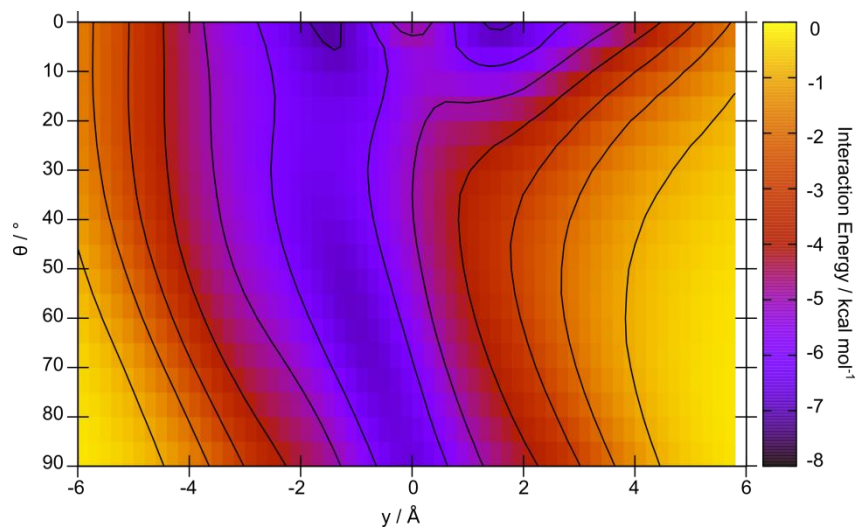


Figure S6. B3LYP-D3/6-31G(d) calculated interaction energies for dimers during molecular rotation and short axis displacement in a naphthalene dimer. Interaction energies were calculated as the difference between the energy of the dimer and the energy of two isolated monomers.