Aviyente Computational Chemistry Group

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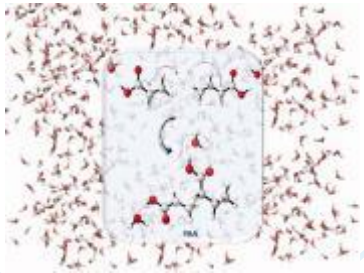
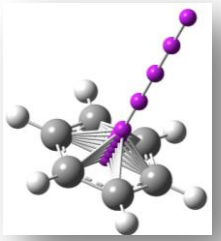
Free Radical Polymerization



Tuğba Furuncuoğlu Özaltın
Berkahan Kura

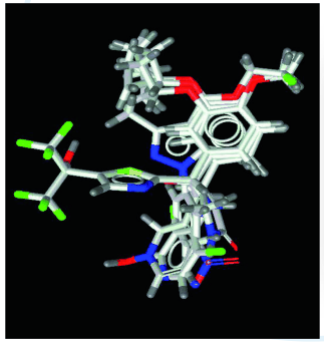
Binding on NMDA Receptors

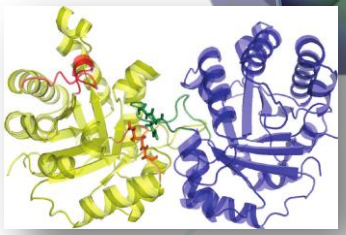


Gamze Bahadır

Research Interests

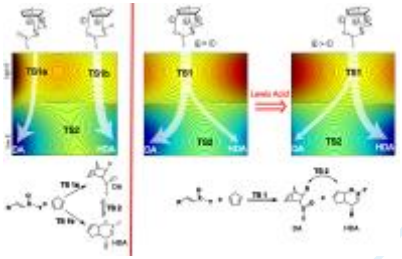
Molecular Docking, Reactions in Proteins and Enzymes





Gülşah Çiftci
Deniz Akgül

Selectivity In Pericyclic Reactions

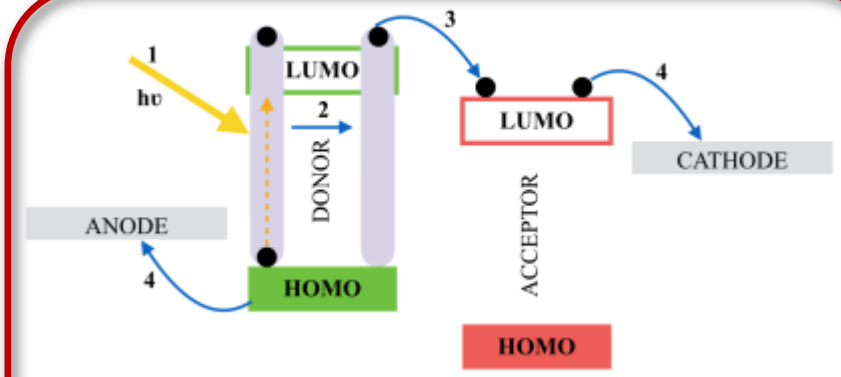


Sesil Agopcan
Burcu Dedeoğlu

ORGANIC PHOTOVOLTAIC CELLS

Tuğçe G. Erbay
Nurdan Merakli

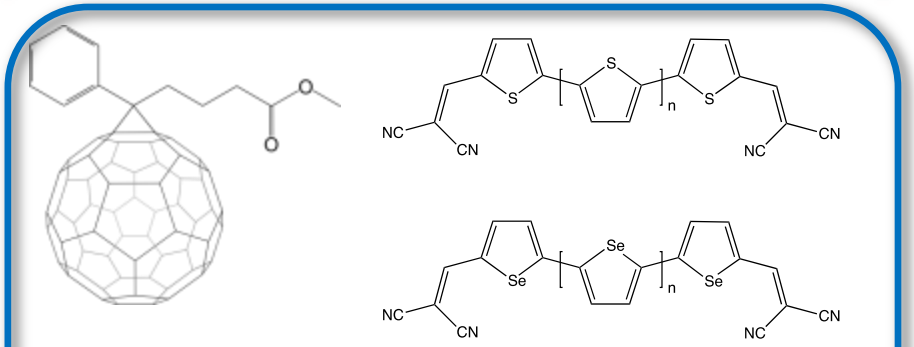
Donor Materials in Organic Photovoltaic Cells



Charge Transfer Mechanism

Aim:

- To improve and develop methods to predict properties of components in OPV cells and to achieve significant improvements in efficiencies of OPV devices.
- Study model oligomer systems, which have good potential to combine the advantages of performance, processability, and are simple for theoretical prediction.



Acceptor

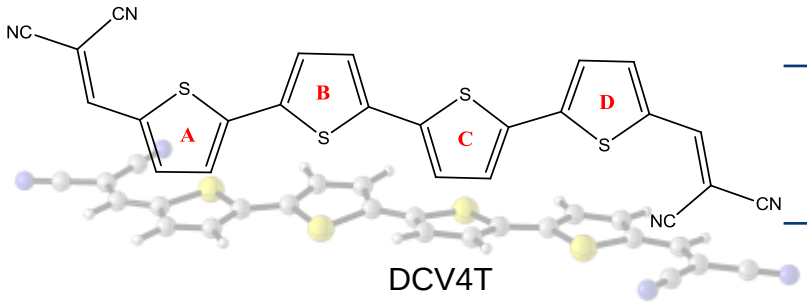
Donor

Acceptor and Donor Materials

Methodology:

- DFT and TDDFT with the M06-2X, B3LYP, B3LYP, ωB97XD and CAM-B3LYP functionals.

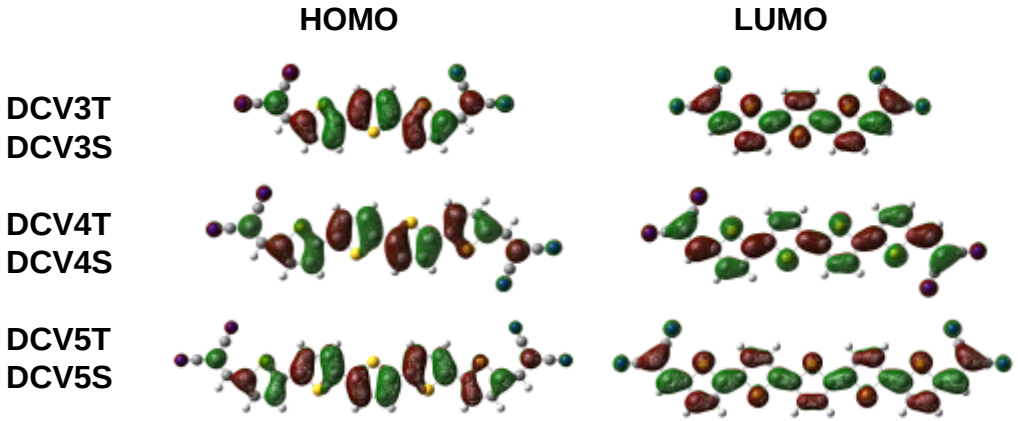
Geometry, Frontier Orbitals, TD-DFT



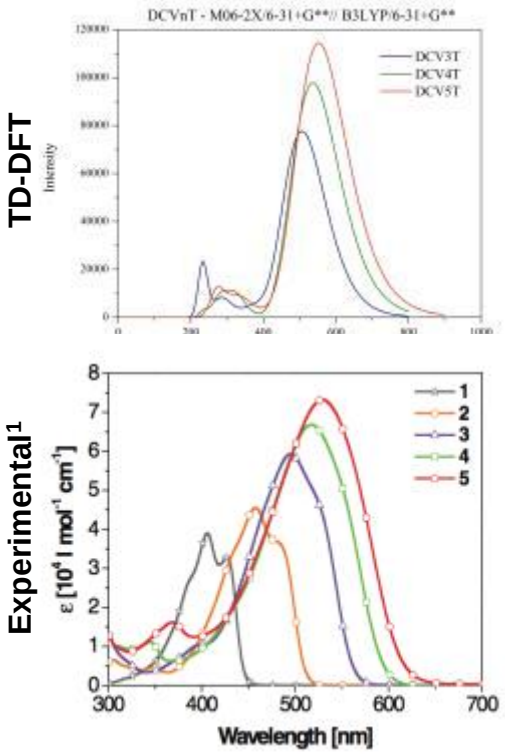
DCV4T

Bond Length Alternation

6-31+G**	B3LYP	ωB97XD	M06-2X	CAM-B3LYP	Exp.1,2
DCV4T	0.035	0.055	0.08	0.054	0.045
DCV4S	0.033	0.055	0.051	0.053	0.051



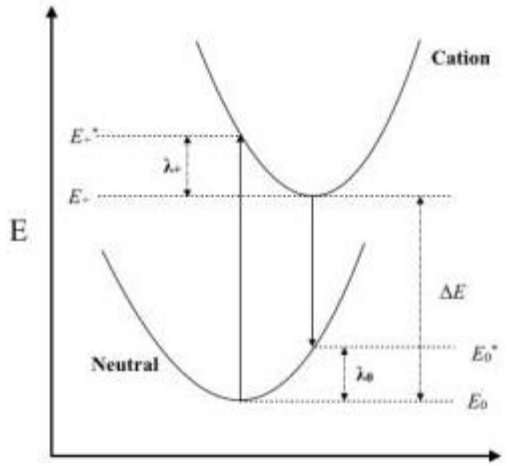
Frontier Orbitals



Absorption Spectra

[1] Fitzner, R., Reinold, E., Mishra, A., Osteritz, E., Ziehlke, H., Körner, C., Leo, K., Riede, M., Weil, M. Tsaryova, O., et al., Advanced Functional Materials, Vol. 21, pp. 897–910, 2011.
[2] Haid, S., Mishra, A. Weil, M., Uhrich, C., Pfeiffer, M., and Bäuerle, P. Advanced Functional Materials, Vol. 22, pp. 4322–4333, 2012.

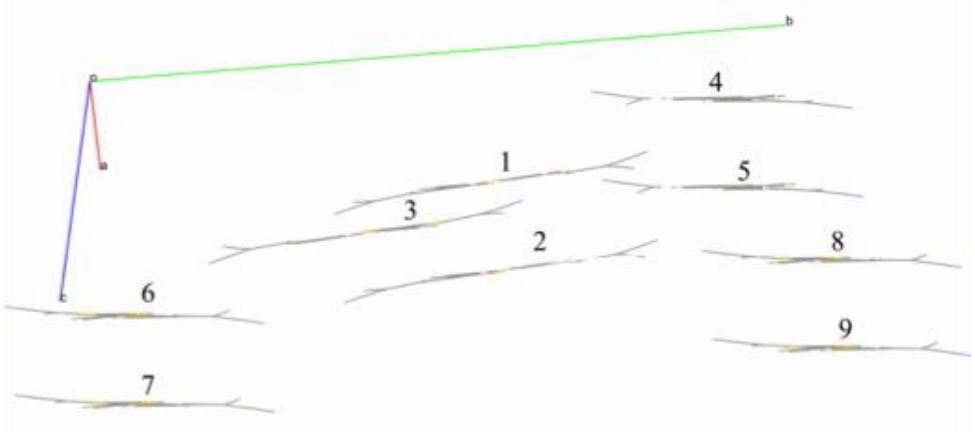
Reorganization Energies & Charge Transport



Reorganization Energies

Table 2. Reorganization Energies

(meV)	λ (Hole)	λ (Electron)
DCV3T	176	275
DCV4T	201	257
DCV5T	196	218
DCV3S	188	278
DCV4S	193	253
DCV5S	196	227



Crystal Packing Structure [1, 2]

Table 3. Transfer integrals

	DCV4T		DCV4S	
Dimer	**t (Hole)**	**t (Electron)**	**t (Hole)**	**t (Electron)**
1_2	-62.787	34.383	-88.097	48.498
1_3	-3.461	12.149	-2.9	9.426
1_5	-2.775	0.881	-2.524	0.908
2_3	12.822	-39.438	12.962	-42.264
2_4	-0.137	0.553	-0.117	0.643
2_5	4.083	6.938	3.414	6.991
4_6	0	0	0	0
5_8	-8.311	-25.092	-10.74	-15.964

[1] Fitzner, R., Reinold, E., Mishra, A., Osteritz, E., Ziehlke, H., Körner, C., Leo, K., Riede, M., Weil, M. Tsaryova, O., et al., Advanced Functional Materials, Vol. 21, pp. 897–910, 2011.
[2] Haid, S., Mishra, A. Weil, M., Uhrich, C., Pfeiffer, M., and Bäuerle, P. Advanced Functional Materials, Vol. 22, pp. 4322–4333, 2012.

COST action no MP1307
Action title:
Stable Next Generation Photovoltaics:Unraveling degradation mechanisms of Organic Solar Cells by complementary characterization techniques (StableNextSol)

- **Plausible contributions**

- Model the effect of water and oxygen in the degradation of small molecule organic photovoltaic devices.

- Understand the impact of charge transfer complexes in the degradation of small molecule organic photovoltaics.

- Test computationally degradation mechanisms already suggested and rank them based on the activation energy barriers.

- Others?