Quantum coherent energy and charge transfer in photovoltaic materials

Antonietta De Sio

Institut für Physik, Carl von Ossietzky Universität Oldenburg

antonietta.de.sio@uni-oldenburg.de



Solar energy conversion in OPV...

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Conversion of solar energy conversion into electricity with organic materials (OPV)



www.heliatek.de

www.epfl.ch

- OPV materials: abundant, non-toxic, color-tunable
- OPV devices: low cost production, flexible, large area devices
- ...but low efficiencies

-MA-

Organic solar cells

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universität | O L D E N B U R G



- Light absorption \rightarrow exciton formation
- Exciton transport to donor-acceptor interface
- Exciton dissociation via photoinduced charge transfer
 → spatially separated charges
- Transport to the respective electrodes
- Charge extraction → current!







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P3HT:PCBM - prototypical OPV blend



Selective excitation of the donor triggers coherent vibrations of the acceptor!

S.M. Falke et al. Science 344, 1001 (2014)



Dynamics

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Coherent charge oscillations between donor and acceptor driven by strongly coupled vibrational motion



S.M. Falke et al. Science 344, 1001 (2014)



OPV and conical intersections

When many vibrations strongly couple to the electronic system...**conical intersections** may form



- CoIns: strong coupling of electrons and vibrations → ultrafast surface crossing
- Theory predicts that CoIns:
 - are ubiquitous in molecules
 - determine ultrafast dynamics and yields of energy and charge transfer processes...

Do they exist in OPV? Are they relevant?

Chemical Reviews 117, 12165, (2017)



OPV and conical intersections

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First experimental signatures of wavepacket motion though an intermolecular CoIn in an OPV material

E. Sommer et al, in preparation (2019)



Relevant for devices?

Particle-like hopping between disordered localized sites

Acceptor

 \rightarrow slow and lossy tranport...



Wavepacket propagation

→ ultrafast and efficient...as long as coherence survives



Relevant for devices?

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Can we **exploit quantum transport** to make solar cells more efficient?

Tailor electron-vibrational coupling:

→ control efficiency of initial charge outcome

 \rightarrow improve device performance

Highly interdisciplinary: ultrafast spectroscopy, quantum dynamics modeling, chemistry, material science, ...



S.M. Falke et al. Science 344, 1001 (2014) A. De Sio et al., Nature Comm. 7, 13742 (2016) A. De Sio, C. Lienau, PCCP 19, 18813 (2017) A. De Sio et al, EPJB 91, 236 (2018) E. Sommer et al, in preparation (2019)



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Work in Oldenburg

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Bremen BCCM. Center for Computational Materials Scie

Thank you for your attention!

