## The 907<sup>th</sup> IMS colloquium

## Molecular understanding of organic-organic interfaces and mixtures



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Date & Time: 2017/6/29 (Thu.) 16:00-Place: IMS Research Building Room 201

We show how inclusion of mesoscale order resolves the controversy between experimental and theoretical results for the energy-level profile and alignment in a variety of photovoltaic systems, with direct experimental validation [1,2]. We explain how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase [2]. Comparing several of smallmolecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices. By accounting for long-range mesoscalefields, we obtain the

ionization energies in both crystalline [3] and mesoscopically amorphous systems with high accuracy [4].

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- 2. C. Poelking, D. Andrienko, J. Am. Chem. Soc., 137, 6320, 2015.
- M. Schwarze, W. Tress, B. Beyer, F. Gao, R. Scholz, C. Poelking, K. Ortstein, A. A. Guenther, D. Kasemann, D. Andrienko, K. Leo, Science, 352, 1446, 2016.
- 4. C. Poelking, D. Andrienko J. Chem. Theory Comput., 12, 4516, 2016.





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