

Workshop I: Solar Cells

Monday September 23, 2013

- 8:00–9:00 *Check-In/Light Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Scheffler*
- 9:00–9:15 *Welcome and Opening Remarks*
- 9:15–9:55 **Mark E. Thompson** (University of Southern California (USC))
New Materials and Insights Into Organic Photovoltaics
- 10:15–10:30 *Break*
- 10:30–11:10 **Brett Savoie** (Northwestern University)
Opportunities (and Challenges) for Photovoltaics on the Mesoscale
- 11:30–11:45 *Break*
- 11:45–12:25 **Karsten Hannewald** (Humboldt-Universität)
Polaron Transport in Organic Crystals: Theory and Modelling
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Giustino*
- 2:30–3:10 **Leor Kronik** (Weizmann Institute of Science)
Frontier Orbitals and Charge Transfer Excitation Energies from Density Functional Theory
- 3:30–4:00 *Break*
- 4:00–4:40 **Jeff Neaton** (Lawrence Berkeley Laboratory)
Excited States and Energy Conversion in Organic Semiconductors from First Principles
- 5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday September 24, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Wei*
- 9:00–9:40 **Annabella Selloni** (Princeton University)
Polaronic states in TiO₂
- 10:00–10:15 *Break*

(Tuesday schedule continued on next page)



(Tuesday schedule continued from previous page)

- 10:15–10:55 **Efthimios (Tim) Kaxiras** (Harvard University)
Modeling of charge transfer rates in hybrid photovoltaics
- 11:15–11:30 *Break*
- 11:30–12:10 **Keith Promislow** (Michigan State University)
Separator membranes for dye sensitized solar cells: the role of nanomorphology
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Galli*
- 2:30–3:10 **Claudia Draxl** (Humboldt-Universität)
Computational concepts for organic/inorganic solar cells combining DFT and many-body perturbation theory
- 3:30–4:00 *Break*
- 4:00–4:40 **Feliciano Giustino** (University of Oxford)
Energy-level alignment at donor/acceptor interfaces for nanostructured solar cells

Wednesday September 25, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Kaxiras*
- 9:00–9:40 **Maria Antonietta Loi** (Rijksuniversiteit Groningen)
Towards highly efficient PbS nanocrystal solar cells
- 10:00–10:15 *Break*
- 10:15–10:55 **Boaz Ilan** (University of California, Merced (UC Merced))
Modeling light propagation in luminescent solar concentrators
- 11:15–11:30 *Break*
- 11:30–12:10 **Nate Lewis** (California Institute of Technology)
A Technical and Operational Perspective on the DOE Energy Innovation Hub in Fuels from Sunlight, the Joint Center for Artificial Photosynthesis
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Kronik*
- 2:30–3:10 **Xiaoyang Zhu** (Columbia University)
Schrödinger's cat and solar energy conversion beyond the limit
- 3:30–4:00 *Break*
- 4:00–4:40 **Gergely Zimanyi** (University of California, Davis (UC Davis))
Transcending QCD in nanostructured solar cells

Thursday September 26, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Promislow*
- 9:00–9:40 **Sergei Tretiak** (Los Alamos National Laboratory)
Life of photoexcited conjugated chromophores: the movie
- 10:00–10:15 *Break*
- 10:15–10:55 **Yang Yang** (University of California, Los Angeles (UCLA))
- 11:15–11:30 *Break*
- 11:30–12:10 **Irene Gamba** (University of Texas at Austin)
Reaction-transfer dynamics in semiconductor-electrolyte solar cells
- 12:45–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Neaton*
- 2:30–3:10 **Michael Chabynic** (University of California, Santa Barbara (UC Santa Barbara))
Structural Order and Interfaces in Organic Solar Cells
- 3:30–4:00 *Break*
- 4:00–4:40 **Carlos Garcia-Cervera** (University of California, Santa Barbara (UC Santa Barbara))
Numerical advances in Self-Consistent Field Theory simulations of block copolymers: Applications to polymer lithography and evaporation-driven pattern selection

Friday September 27, 2013

- 8:00–9:00 *Continental Breakfast*
- 9:00 *Session Chair: Draxl*
- 9:00–9:40 **Clas Persson** (University of Oslo)
Properties of Cu(In,Ga)Se₂ absorber material
- 10:00–10:15 *Break*
- 10:15–10:55 **Su-Huai Wei** (National Renewable Energy Laboratory)
Defect Control of Kesterite Cu₂ZnSn(S,Se)₄ for Thin-film Solar Cell Absorbers
- 11:15–11:30 *Break*
- 11:30–12:10 *Wrap Up Discussion*

