

Program of Seminar at Chicheley Hall

March 23-25, 2022 Chicheley Rd, Newport Pagnell MK16 9JJ, UK

Day 1: 23rd March 2022

Welcome and Introduction

10:00-10:45 Coffee

10:45-11:00 **Jochen Blumberger** Welcome

Section 1 Chair: Jochen Blumberger

11:00-11:35 **Artem Bakulin, Imperial College London**
Time-resolved charge and energy dynamics in organic electronic materials for photovoltaic applications

11:35-11:55 **Wei-Tao Peng, University College London**
Multiple Channels of the Exciton Dissociation in a 1D Fullerene-Oligothiophene Junction: Comparing the MCTDH and FOB-SH Dynamics

11:55-12:15 **Jun Yan, Imperial College London**
Relationship between structure and light absorption strength in organic small molecules

12:15-13:00 **Poster Session 1**

13:00-14:00 Lunch

14:00-16:00 Walk through nearby fields:
<https://my.viewranger.com/route/details/MTM2MTY3Mg==>

16:00-16:30 Coffee

Section 2 Chair: Artem Bakulin

16:30-17:05 **Jenny Nelson, Imperial College London**
Impact of chain conformation on charge transport in conjugated polymers

17:05-17:40 **Samuele Giannini, University of Mons**
Transient delocalization of charge and energy carriers in organic electronic materials

17:40-18:00 **Jarvist Moore Frost, Imperial College London**
Polaron physics within the Feynman variational path integral approach

18:00-19:00 Time for discussions

19:00 Dinner

Day 2: 24th March 2022

Section 3 Chair Roohollah Hafizi

- 09:00-09:35 **Alexander Cowan, University of Liverpool**
Surface and transient spectroscopy of photocatalysts and electrodes
- 09:35-09:55 **Philipp Schienbein, University College London**
Solvation Dynamics at the Hematite/Liquid Water Interface Using Neural Network potentials with Hybrid DFT Accuracy
- 09:55-10:30 **Alexander Rettie, University College London**
Polarons in metal oxide photoelectrodes
- 10:30-10:50 **Chris Ahart, University College London**
Charge mobility in hematite from constrained hybrid density functional theory
- 10:50-11:20 Coffee break

Section 4 Chair: Alexander Cowan

- 11:20-11:55 **Ismael Diez Perez, King's College London**
Bioengineered Single-Protein Electronics
- 11:55-12:15 **Xiaojing Wu, University College London**
Calculation of Electric Currents on single-protein Junctions
- 12:15-13:00 **Poster Session 2**
- 13:00-14:00 Lunch

Social event

- 14:00-17:00 Visit of national computing museum: <https://www.tnmoc.org/>
- 17:00-19:00 Time for discussions
- 19:00 Dinner

Day 3: 25th March 2021

Section 5 Chair: Jenny Nelson

- 09:00-09:35 **Henning Sirringhaus, University of Cambridge**
Experimental evidence for transient localisation in high mobility molecular and polymeric semiconductors
- 09:35-09:55 **Nora Gildemeister, University of Cologne**
Charge transport simulation in merocyanines
- 09:55-10:15 **Ljiljana Stojanovic, University College London**
Charge transport simulation in the nonfullerene acceptor O-IDTBR
- 10:15-10:45 Coffee break

Section 6 Chair: Henning Sirringhaus

- 10:45-11:05 **Jan Elsner, University College London**
Temperature Dependence of the Charge Mobility in Rubrene from FOBSH
- 11:05-11:25 **Roohollah Hafizi, University College London**
Machine learning of electronic couplings of molecular dimers
- 11:25-12:00 Time for discussions
- 12:00-13:00 Outlook: Further Directions & Collaborations
- 13:00-14:00 Lunch (END)

Poster session 1: 12:15-13:00 on 23rd March

Jan Elsner

Roohollah Hafizi

Nora Gildemeister

Ljiljana Stojanovic

Jack Coker

Daniel Garcia Medranda

Poster session 2: 12:15-13:00 on 24th March

Chao Li

Tracy Ha and Jhanelle White

Chris Ahart

Philipp Schienbein

Xiaojing Wu

Participants list

From Imperial College London

Jenny Nelson

Daniel Garcia Medranda

Jack Coker

Jarvist Frost

Jun Yan

Artem Bakulin

Ziming Chen

From King's College London

Ismael Diez Perez

Tracy Ha,

Jhanelle White

From University College London

Jochen Blumberger

Ljiljana Stojanovic

Philipp Schienbein

Chris Ahart

Xiaojing Wu

Jan Elsner

Nora Gildemeister

Roohollah Hafizi

Alexander Rettie

From University of Cambridge

Henning Sirringhaus

Yucheng Xu

From University of Liverpool

Alexander Cowan

Chao Li

From University of Mons

Samuele Giannini