Imperial College London

M-RHEX
Energy Conversion | Capture | Storage

Neutron Scattering for Understanding Energy Materials:
A tutorial workshop

Lecture Theatre 1, Blackett Laboratory
Imperial College London
13 June 2019

Introduced by: Jenny Nelson, Imperial and Paul McMillan, University College London

Meeting organised by:

Dr. Anne Guilbert, Department of Physics, Imperial College London, UK

Dr Fabrizia Foglia, Department of Chemistry, University College London, UK

EPSRC Engineering and Physical Sciences Research Council

Materials research hub for energy capture, conversion, and storage: Vision

Understanding of the broad scientific principles that govern charge motion in novel materials is critical to the establishment of materials design strategies

Fundamental research into charge transport can be relevant across technologies, including batteries, solar cells, and electrochemical conversion devices

Rather than studying materials useful for a single category of device, research can on modes of charge transport (electronic, ionic, mixed) in a cross-cutting way

Consortium:

Oxford (Engineering, Materials, Physics)
Imperial College London (Chemistry, Engineering, Materials, Physics)
University **College London (Chemistry, Engineering)**
Swansea (Engineering)
Coventry (Engineering)

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Materials research hub for energy capture, conversion, and storage: Science

Three key thrusts focus on **fundamental science of conductive materials**

- Porous electrodes and nanostructured-composite ion conductors (Traditional battery electrodes, redox flow reactors, fuel-cell catalysts, etc.)
- Mixed ionic/electronic conductors (Organic and inorganic materials for photon harvesting, SOFC separators, metal/air battery discharge products, SEIs)
- Single-ion conductors, including solid electrolytes and ionomer membranes

One thrust focuses on **challenges of scaleup/translation**

How to make manufacturable structures?
How to assess the utility of the fundamental understanding that develops?

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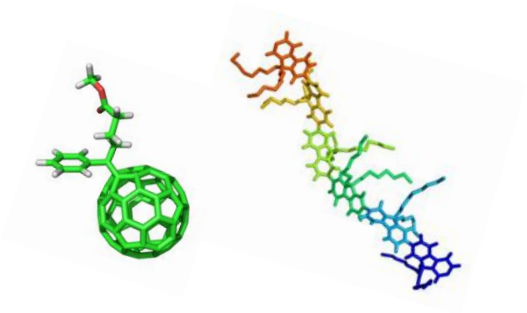
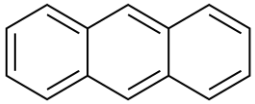
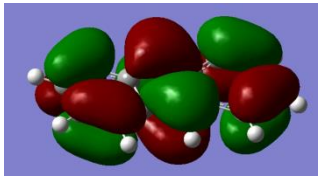
Molecular electronic materials

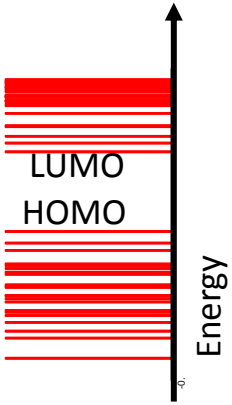


Molecular semiconductors

π conjugation







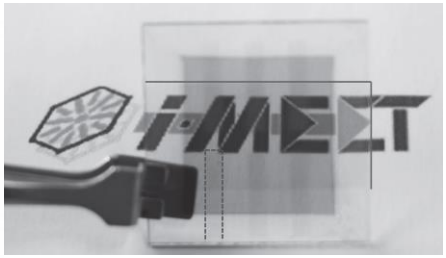
⇨ Tuneable electronic & optical properties

Applications

LG

Light emission

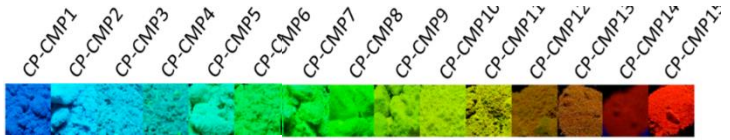
Photovoltaics



Electrochromics

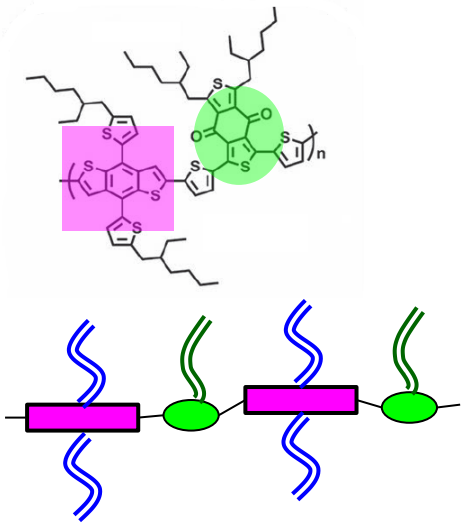
J. Reynolds et al, GATECH

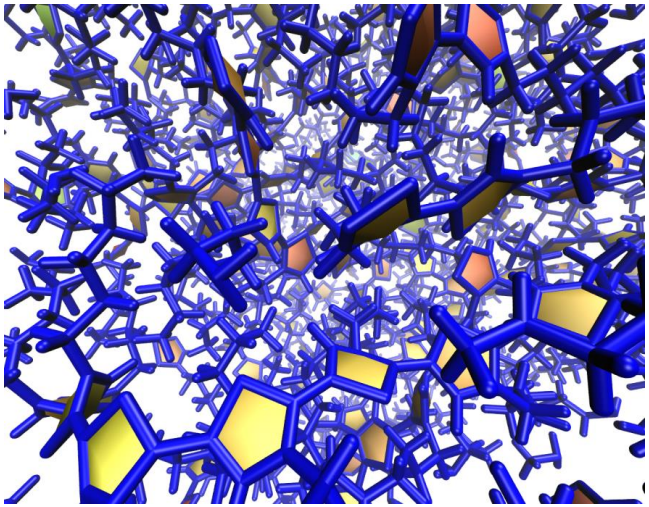
Photocatalysis

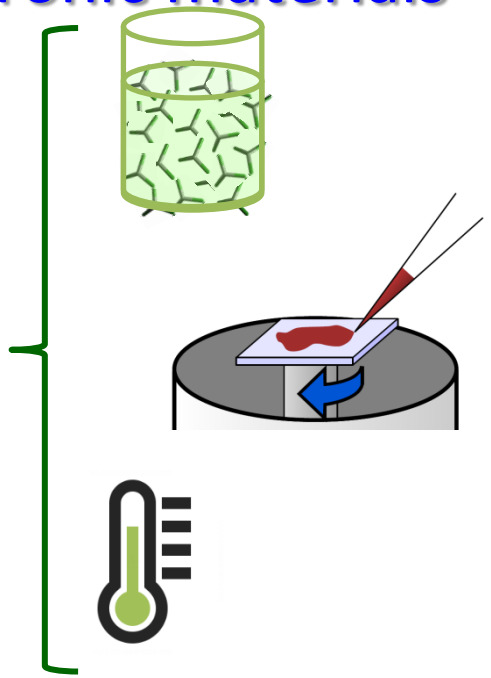


R. S. Sprick et al, JACS 2015

The beauty and the beast in molecular electronic materials







- Redox and optical properties controlled (largely) by molecule or monomer
- Microstructure controlled (largely) by side chains and processing
- Electronic transport controlled by local pairwise interactions and shape
- Processable, cheap and flexible materials

But…

- Electronic properties depend strongly on microstructure and structural dynamics(strong electron-phonon coupling)
- Microstructure is hard to control…
- Microstructure is hard to measure

We need tools to measure and simulate microstructure and its evolution

Role for neutrons as probes of molecular electronic materials

- **Neutron diffraction** → structural information on ordered parts of system
- **Neutron reflectometry** → information on the structure of layered system
- **Small angle neutron scattering** → structure adopted by polymer chains or aggregates e.g. in solution
- **Inelastic neutron scattering** → energies of low-frequency vibrational modes of molecules and assemblies
- **Quasi-elastic neutron scattering** (QENS) → dynamics of motions of polymer chains and side chains

- Advantages:
  - QENS and INS can probe the amorphous part of the sample volume (i.e. the larger and more relevant part!)
  - No optical selection rules: all modes are visible
  - High penetration depth (not only a surface technique)
  - Flexibility to use hetero-isotopes to enhance or mask components

H. Cavaye, Angew. Chem. Int.Ed. DOI: 10.1002/anie.201812950

Role for neutrons as probes of molecular electronic materials

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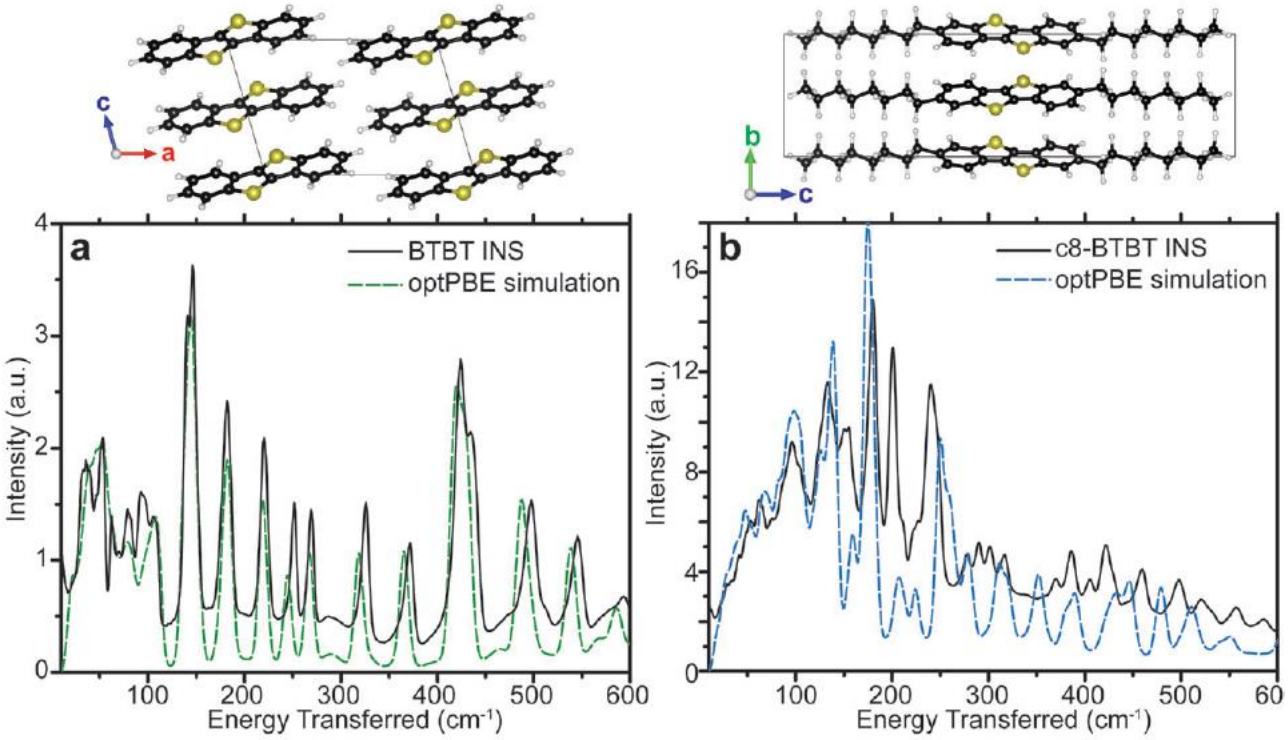


Low energy phonon modes of organic crystals measured by INS.

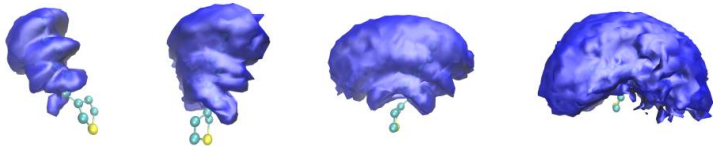
Calculated modes used in a model of hole mobility (based on dynamic fluctuations in coupling)

T. F. Harrelson et al., Mater. Horiz. 2019 DOI: 10.1039/c8mh01069b

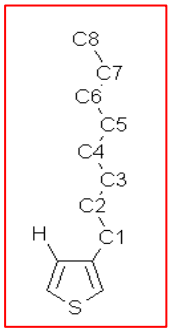
Role for neutrons as probes of molecular electronic materials

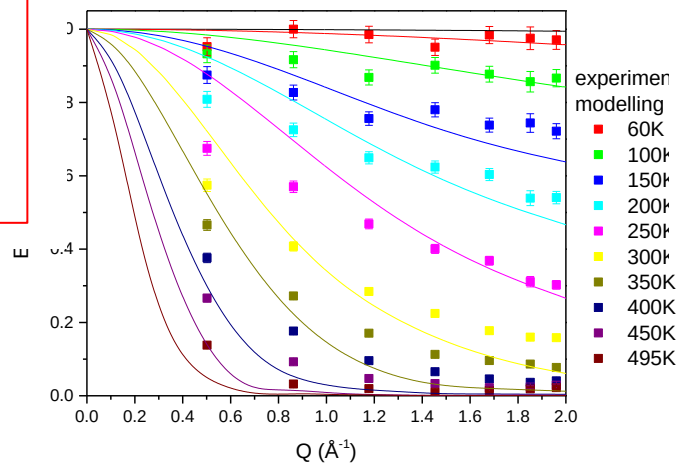
- **Quasi-elastic neutron scattering** (QENS) → dynamics of motions of polymer chains and side chains

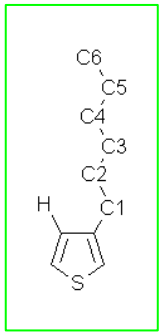
molecular dynamics:

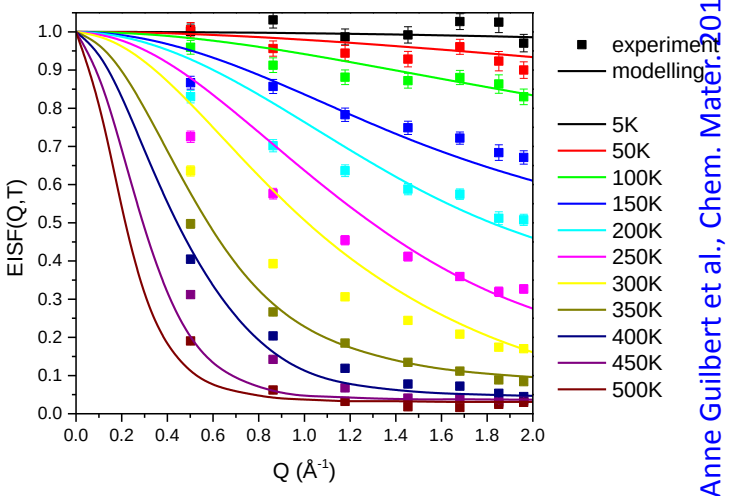


Increasing temperature









Simulation of temperature dependent structure factor using atomistic molecular dynamics serves to validate the MD force fields and approach

Anne Guilbert et al., Chem. Mater. 2015, DOI: 10.1021/acs.chemmater.5b03001

Neutron Scattering for Understanding Energy Materials

- **10:30** Neutrons and energy materials: introduction and applications (Prof Jenny Nelson (Imperial College London) and Prof Paul F McMillan (University College London))
- **10:45** Neutrons at ISIS (Dr Victoria Garcia Sakai; ISIS, Didcot, UK)
- **11:15** Neutrons at ILL (Dr Mohamed Zbiri; Grenoble, France)
- **11:30** Ion dynamics in fuel cell battery materials by QENS (Dr Sandrine Lyonnard; CEA, Grenoble, France)
- **12:00** Lunch Break
- **13:00** Neutron Reflectivity for energy applications (Dr Maximilian Skoda; ISIS, Didcot, UK)
- **13:30** Photo-excited polymers in matrices (Dr Anne A Y Guilbert; Imperial College London, UK)
- **14:00** QENS: from scattering profile to dynamical parameters (Dr Fabrizia Foglia; University College London, UK)
- **14:30** Coffee Break
- **14:45** Small-angle neutron scattering for structure, composition and thermodynamics in polymer blends and energy materials (Dr Alisyn Nedoma; University of Sheffield)
- **15:15** Molecular behaviour in porous catalysts (Dr Alexander O'Malley; University of Bath, UK)
- **15:45** Discussion