

# NLS Chemical Sciences Workshop

NLS Workshop 22nd-23rd May 2008

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# Executive Summary

- STFC seeks to examine the case for a New Light Source Facility in the UK with unique and world leading capabilities
- The proposal is jointly supported by STFC and Diamond Light Source Ltd, coupled to strong HEI involvement
- The first phase is broad-based science consultation
  - Workshops and Working Groups coordinated by the leaders of the “Photon Science Research Institute” and the 4GLS project
  - Direct input from anyone in the community

# Science Consultation

- The first phase of the NLS project will determine, through wide consultation, the key long term scientific objectives for the UK light source strategy and establish the light source capability we need
  - *“What is the compelling science?”*
- NLS will examine the balance between objectives which can be achieved by exploiting the existing array of international next generation light sources and those which will require a new UK capability
  - *“Do we need a new UK source?”*

# What is NLS?

- A science driven project
  - First: define the key science drivers
  - Next: assess the technical solution
  - Then: assess funding and location
- Must take the long view of high level objectives that are likely to be relevant for decades
- The NLS facility, if built, will probably adopt an integrated approach;
  - e.g. incorporating advanced conventional lasers alongside FEL(s) to achieve the science objectives

# Establishing Key Science Drivers and Outline Specifications - the Workshops

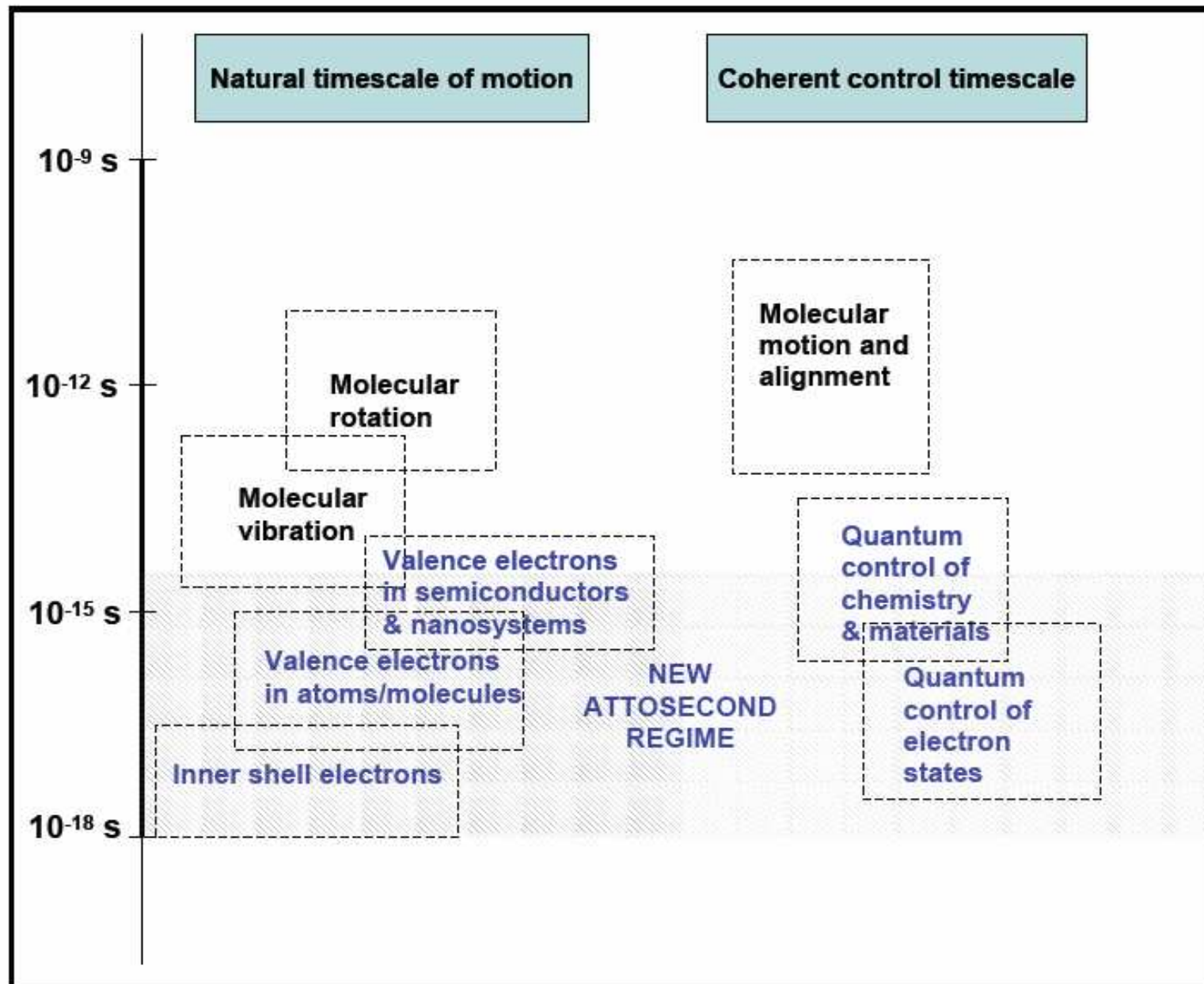
- Electron Dynamics / Attosecond Science\*
  - 13th May 2008, Imperial College London
  - Meeting convenor – Professor Jon Marangos
- High Energy Density Science
  - 20th May 2008, Rutherford Appleton Laboratory
  - Meeting convenor – Professor Justin Wark
- Condensed Matter\*
  - 21st May 2008, Rutherford Appleton Laboratory
  - Meeting convenor – Professor Andrea Cavalleri
- **Chemical Science [ \* areas of strong overlap ]**
  - **22-23rd May 2008, Daresbury Laboratory**
  - **Meeting convenors – Dr. Jonathan Underwood and Professor Wendy Flavell**
- Advanced Photon Sources\*
  - 3rd June 2008, Daresbury Laboratory
  - Meeting convenor – Professor Richard Walker
- Life Sciences\*
  - Workshop June 19<sup>th</sup> , Rutherford Appleton Laboratory/ Diamond Light Source
  - Meeting convenors– Professor Dame Louise Johnson and Professor Peter Weightman

# Chemical Science Objectives?

- To probe the dynamics and mechanism of chemical change
- To understand coupled flow of energy and charge in molecules
- To understand dynamics in complex environments
- To design new active electronic/optical devices, catalysts, functional materials, clean energy sources
- To control chemical processes through rational and targeted design
- To control chemical processes using light

# 4GLS flagship chemical science groups

- Quantum chemical control
- Origins
  - Spectroscopy of transient atoms, molecules and ions, EBIT, ultracold chemistry, gas grain chemistry, single nanoparticle chemistry
- Reaction pathways in catalytic chemical processes
- Reaction dynamics of excited states and free radicals in chemistry & biology (RESRAD)



# Input to NLS Specification

Science Workshops and Working Groups must address and define the desired source parameters for each science area:

- photon energy range(s)
- pulse energy
- pulse length/bandwidth
- pulse/macropulse repetition rate
- average flux/brightness
- degree of coherence
- polarization
- stability in energy, intensity, timing, position
- contrast against background
- requirement for combinations of sources (e.g. THz, IR, SR, electrons etc.) and degree of synchronisation .... etc.

+ State of the art “conventional” lasers and NLO

# Workshop Programme

Thursday 22nd May

- 10:15 Arrive, coffee
- 10:30 Introduction: Jonathan Underwood & Wendy Flavell
- 10:45 Prof Andreas Wolf (Max-Planck-Institut fuer Kernphysik)
- 11:15 Prof Ivan Powis (University of Nottingham)
- 11:45 Discussion
- 12:15 Lunch
- 13:15 Prof Mike Ashfold (University of Bristol)
- 13:45 Prof Richard Catlow (University College London)
- 14:15 Coffee
- 14:45 Prof John Evans (University of Southampton)
- 15:15 Prof Simon Pimblott (University of Manchester)
- 15:45 Discussion
- 16:45 End

# Workshop Programme

Friday 23rd May

- 10:15 Arrive, coffee
- 10:30 Introduction: Jonathan Underwood & Wendy Flavell
- 10:45 Prof Christian Bressler (Ecole Polytechnique Federale de Lausanne)
- 11:15 Prof Sven Shroeder (University of Manchester)
- 11:45 Discussion
- 12:15 Lunch
- 13:15 Dr David Townsend (Heriot Watt University)
- 13:45 Prof Helen Fielding (University College London)
- 14:15 Coffee
- 14:45 Prof Martin McCoustra (Heriot Watt University)
- 15:15 Discussion
- 16:15 End

# Discussion essential to this process

## – we need to hear your views

- Please e-mail directly to us:
  - [j.underwood@ucl.ac.uk](mailto:j.underwood@ucl.ac.uk)
  - [wendy.flavell@manchester.ac.uk](mailto:wendy.flavell@manchester.ac.uk)
  - [j.marangos@imperial.ac.uk](mailto:j.marangos@imperial.ac.uk)
- Or up-load to website (links to be available shortly) your views and ideas
- If you do raise any points during discussions we will note them – but it would help us if you would also e-mail these later to ensure they are accurately captured