Establishing a Relativistic Ultrafast Electron Diffraction & Imaging (RUEDI) National Facility

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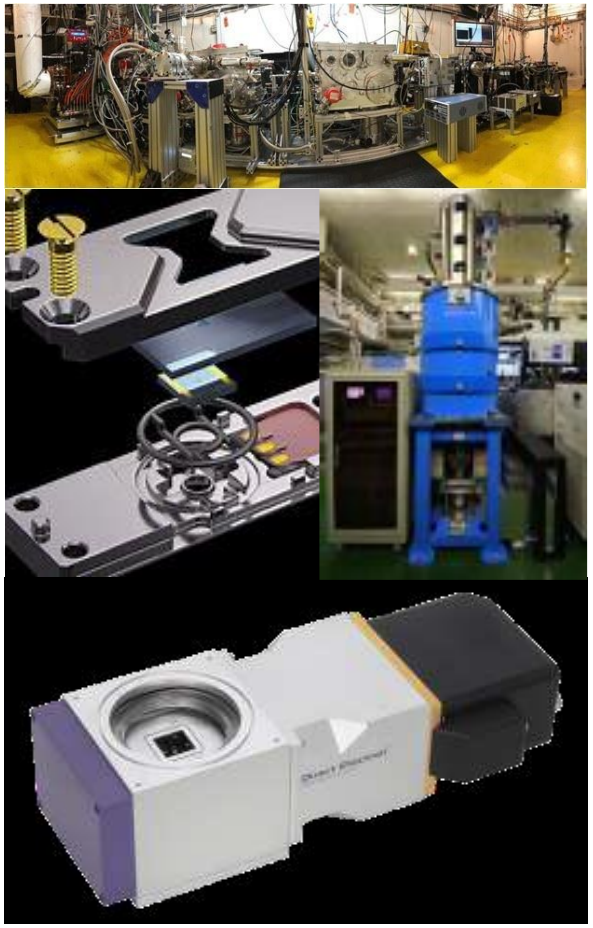
1. University of Liverpool
2. Swansea University
3. STFC- Daresbury
4. Rosalind Franklin Institute
5. University of Toronto
6. University College London
7. University of Leeds
8. Imperial College

What is RUEDI?

A national user facility using MeV electrons for imaging and diffraction on ultrafast timescales



Transformative Science Themes Accelerating UK Technologies

- **Dynamics of Chemical Change**
- **Materials in Extremes**
- **Quantum Materials & Processes**
- **Energy Generation, Storage and Conversion**
- **In Vivo Biosciences**

World leading advances in accelerator, lens, operando stages and detector designs coupled to advances in artificial intelligence

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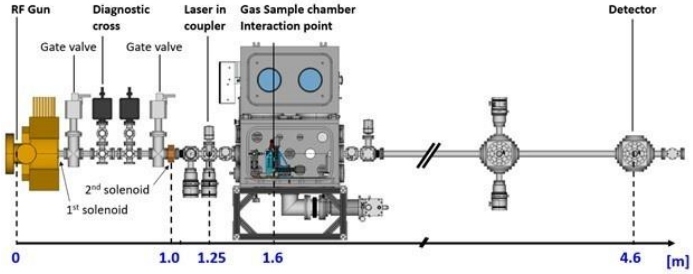
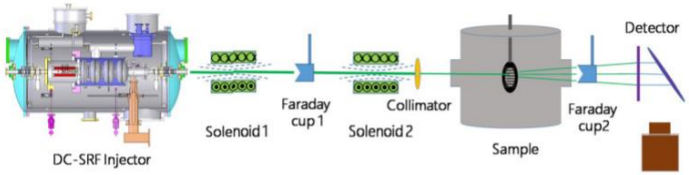
Relativistic UED Facilities Worldwide

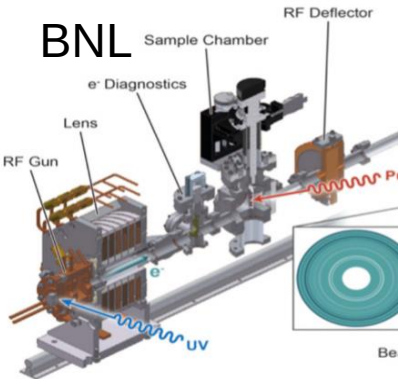
SLAC



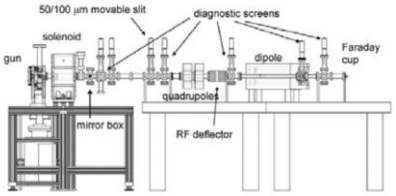
Peking University



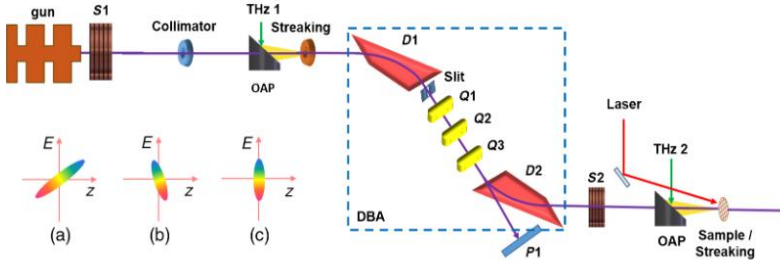
BNL



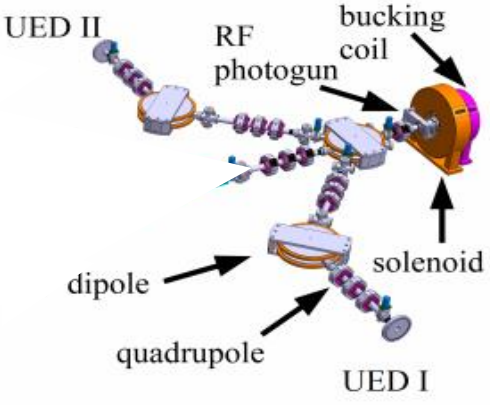
UCLA



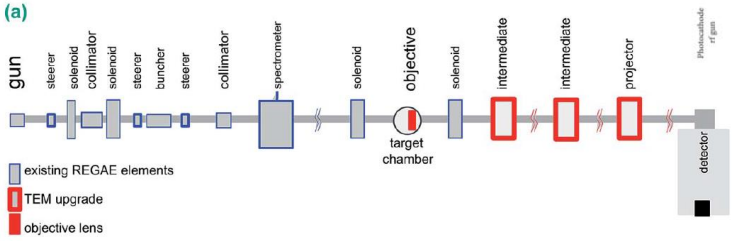
Shanghai



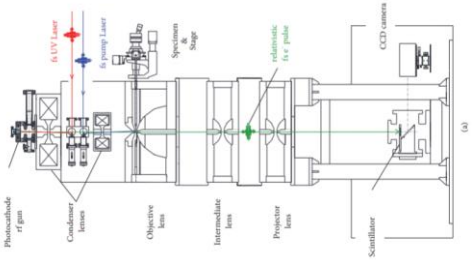
KAERI



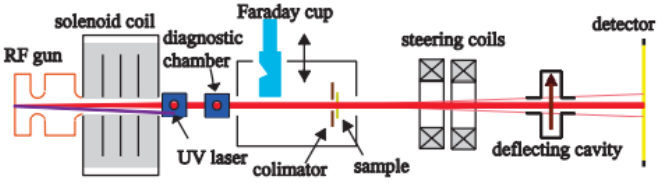
DESY



Osaka



Tsinghua



What Will Make RUEDI Unique?

- **Core Instrument Beyond Femtosecond Ultrafast Electron Diffraction**

  - Imaging dynamics with single electron precision
  - Operando temp, pressure, liquid, mechanical, optical, full rotation
  - Integrated AI for Low-signal image analytics

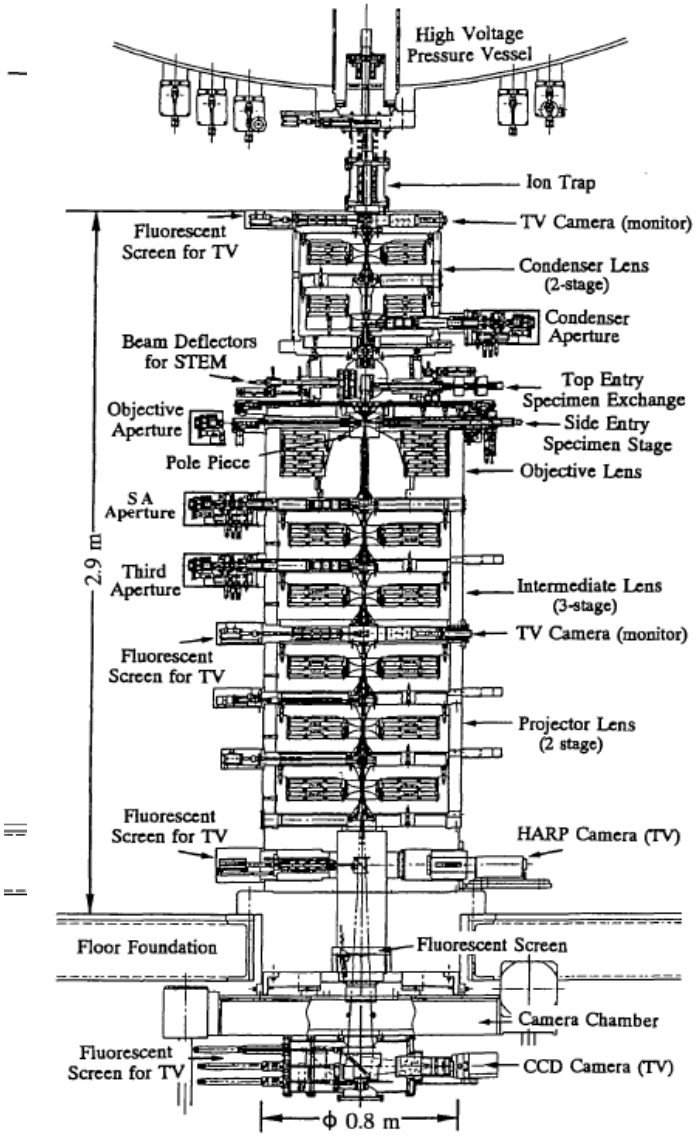
- **Transformative Science Themes tied to EPSRC Prosperity Outcomes**

  - Health innovations through in-vivo biosciences
  - Energy security: generation, transformation, storage
  - Discovery of disruptive materials applications
  - Next generation electronic/magnetic control
  - Materials in extreme conditions
  - AI driven operations

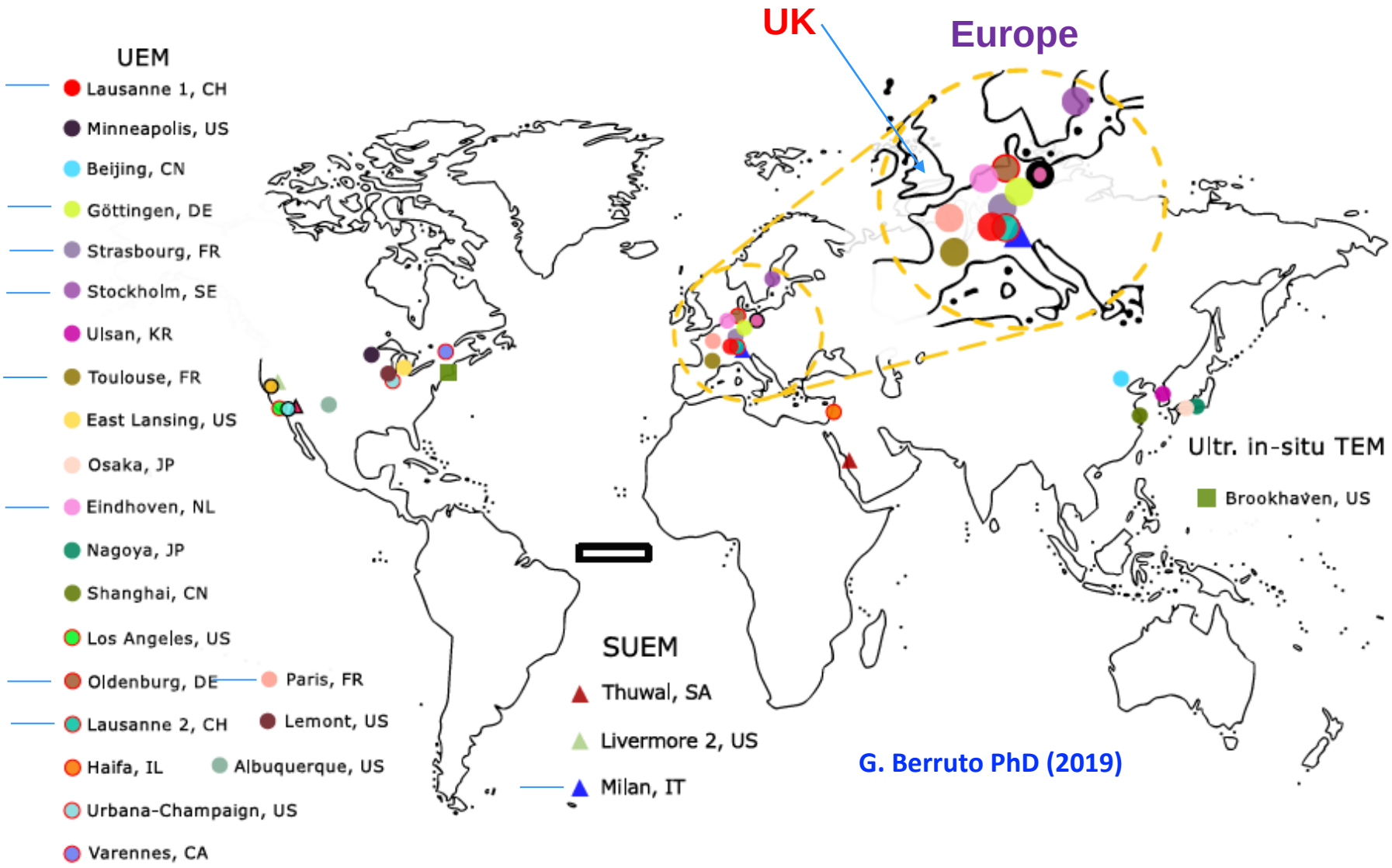
- **Hub and Spoke National Facility**

  - Data driven (intelligent) instrument and user program
  - Comprehensive expertise through hybrid interactions
  - Direct links to industry users and/or partners

10fs diffraction & sub-nm with <100fs imaging



UEM Facilities Worldwide



Leveraging UK Research Infrastructures

-the core team developing the facility

University of Liverpool

The Materials Innovation Factory

Rosalind Franklin Institute

Harwell Campus Hub

STFC Daresbury Laboratory

Cockcroft Institute

Negotiations underway to link access modes and research areas with national institutes and facilities

(anyone interested should let me know)

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The Rosalind Franklin Institute

UKRI Science and Technology Facilities Council

The Management Team - UofL

Director	Research Coordinator	Head of Ops	Administrator	Data Scientist
				
Nigel D. Browning	Yoshie Murooka	Jan Nugara	Lee Kelsall	Alberto Acuto

Responsibility to deliver and operate a national user facility

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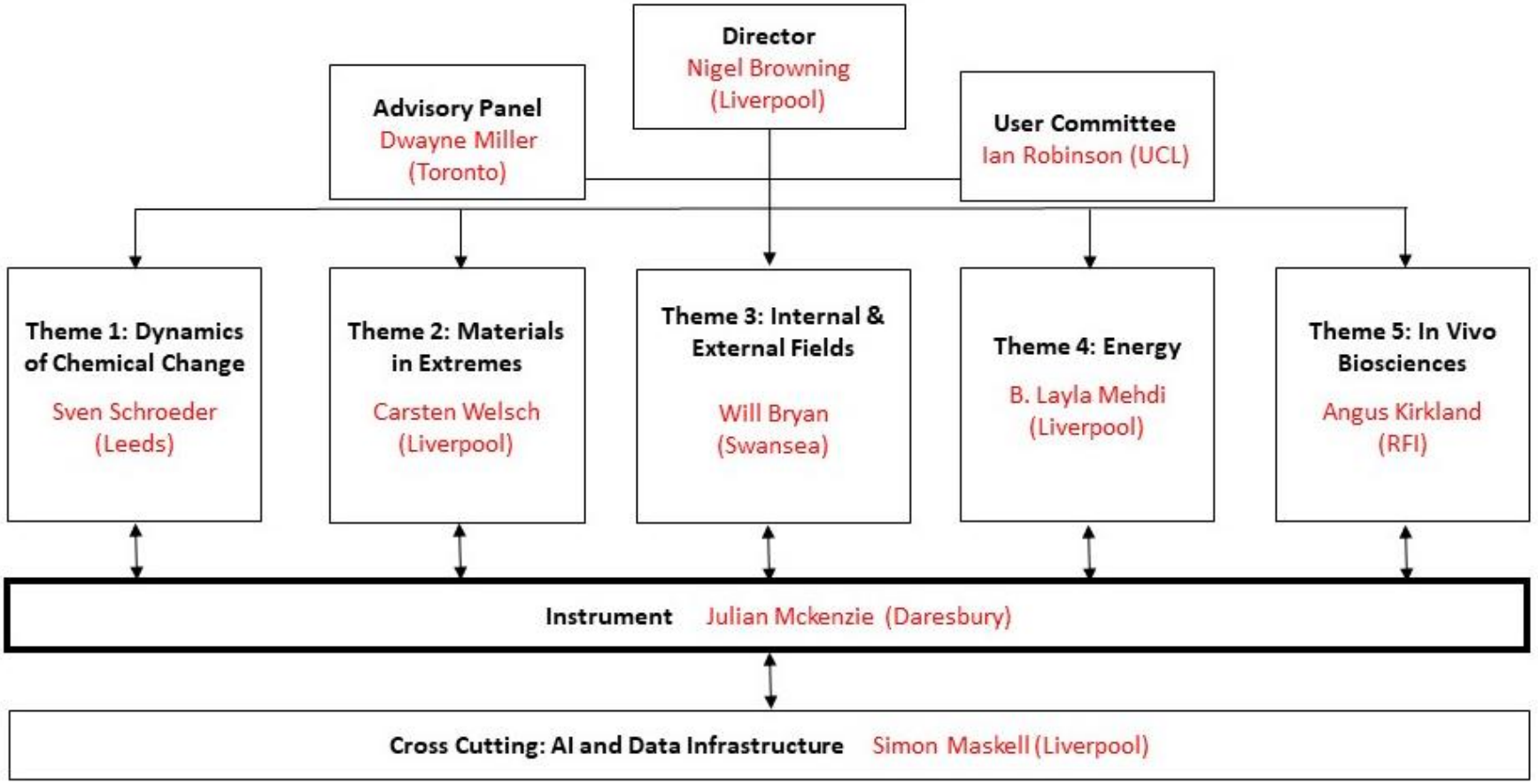
From Concept to User Facility in 5 Years



Soliciting contributions from around the UK to establish high impact science themes

The Instrument Team

Julian McKenzie
Technical Lead

Tim Noakes
Project Sponsor

Mike Ellis
Project Manager

Boris Militsyn
Electron Source

Alan Wheelhouse
RF

Mark Roper
Lasers

Nirav Joshi
Synchronisation

Yuri Saveliev
Diagnostics

Layla Mehdi
Stages

Angus Kirkland
Lenses/Detectors

Clive Hill
Engineering

Graham Cox
Controls

Rachael Buckley
Infrastructure

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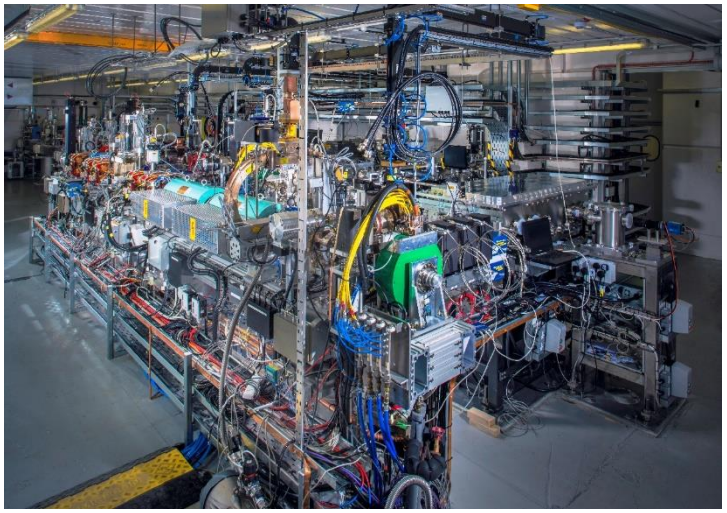
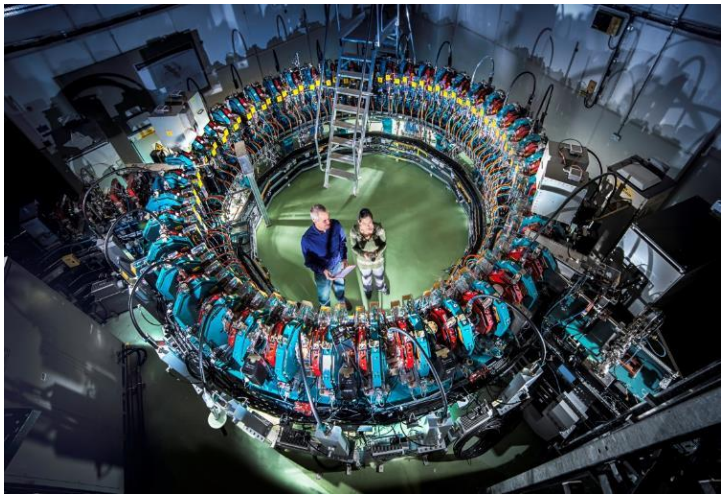
The Rosalind Franklin Institute

UKRI Science and Technology Facilities Council

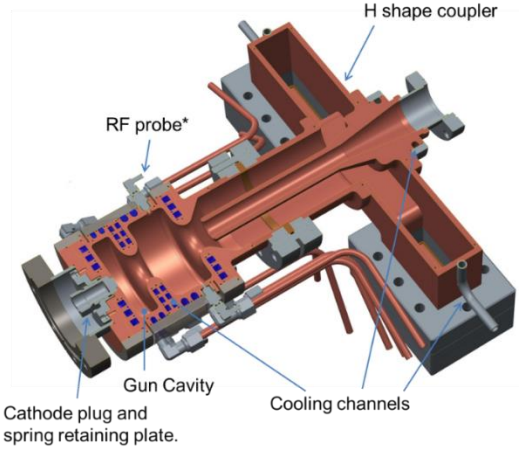
Leveraging STFC Daresbury Expertise

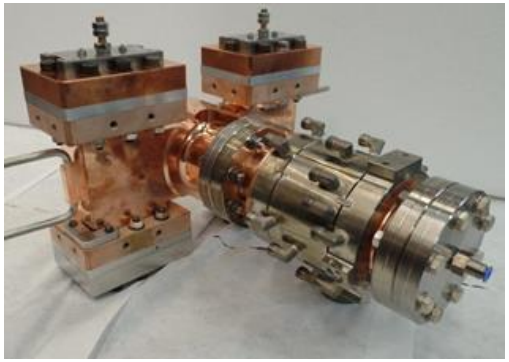
Design, build, and operation of particle accelerator facilities





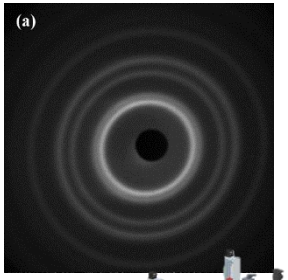
Femtosecond photoinjector development

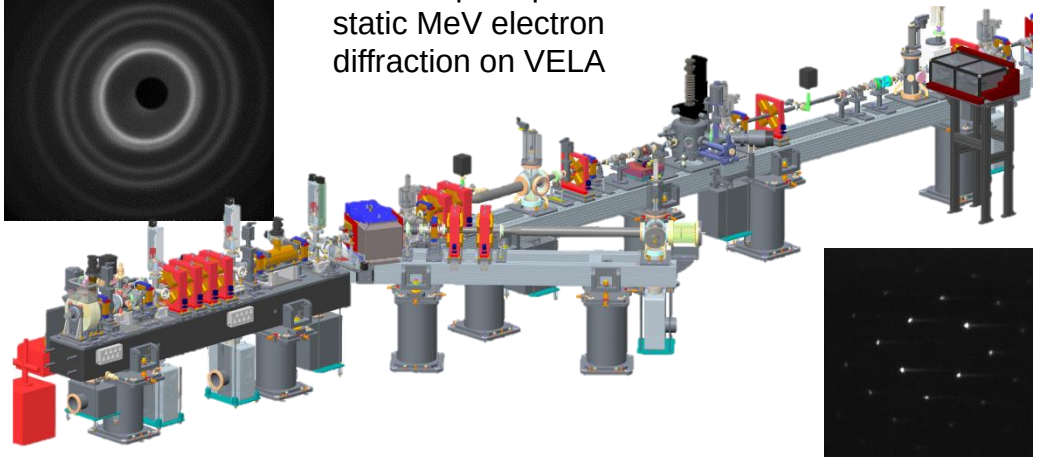




MeV ED experience

Proof-of principle static MeV electron diffraction on VELA





Modes of Operation

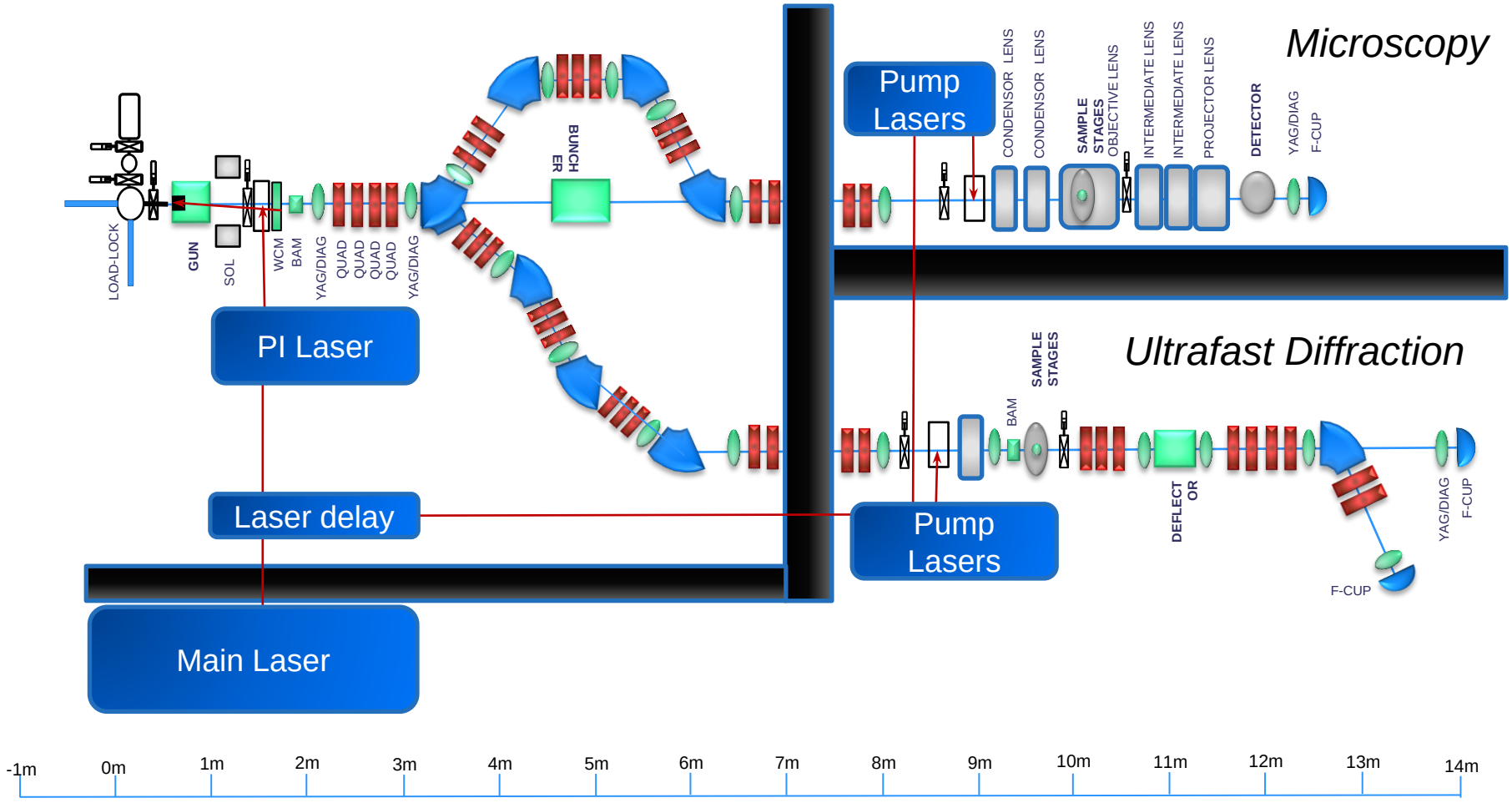
#	Purpose	Electron beam energy	Electrons per bunch	Temporal resolution	Spatial resolution	Spot size
1	**Imaging** *(higher resolution)*	2 MeV	10^6	Few ps	<1nm	
2	**Imaging** *(ultra-fast)*	2 MeV	10^6	<800 fs	~10nm	
3	**Diffraction**	4 MeV	10^6	100 fs		100um
4	**Diffraction** *(low-charge)*	4 MeV	10^4	10 fs		10um
5	**Diffraction** *(Streaking*)*	4 MeV	10^7	10 fs		100um

**streaking mode is single-shot, time-resolved, where the time information implanted onto transverse plane via a deflector/streaker*

Range of pump laser wavelength/durations/intensities

All modes limited to 100Hz repetition rate *(with potential future upgrade to 1kHz)*

RUEDI Schematic 2.0



~£40M, 3 year construction project starting in 2024

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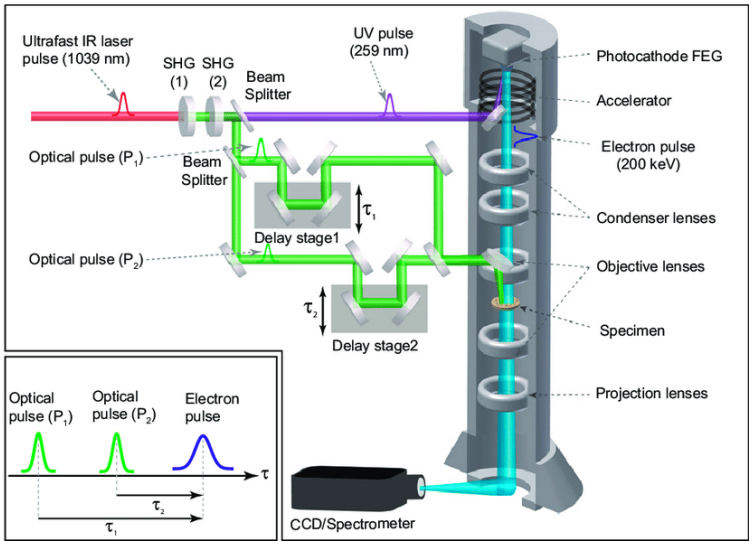
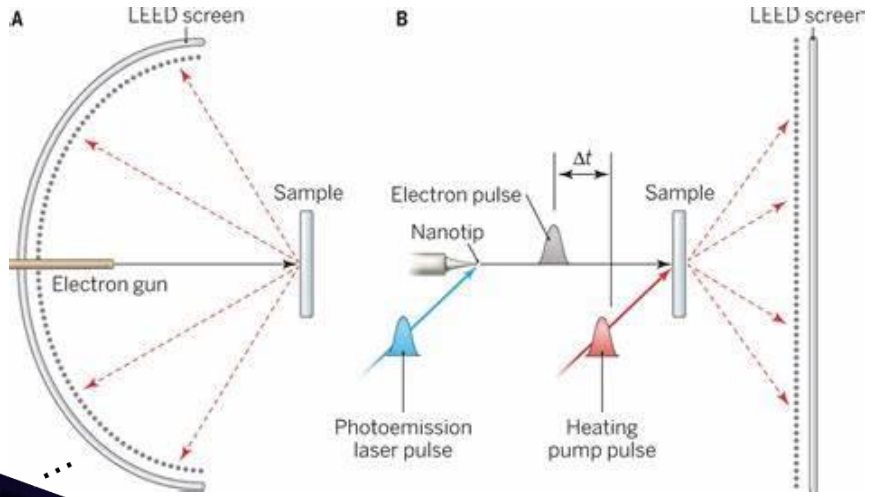
The RUEDI Ecosystem – linked facilities

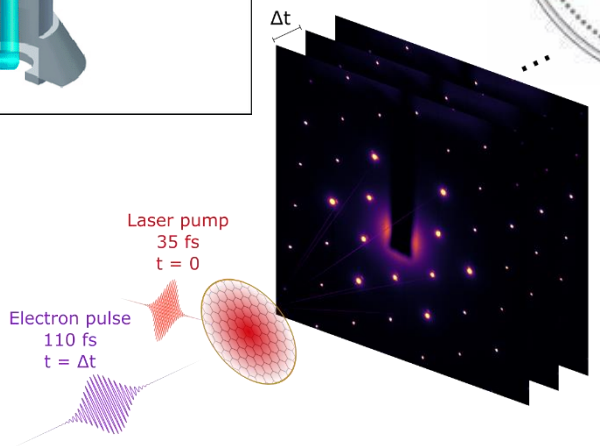
UEM



ULEED/ULEEM



UED



Leveraging partners expertise in instrumentation, imaging, ultrafast methods, lasers, materials science, structural biology

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Science & Cross-Cutting Themes

Materials in Extremes

Carsten Welsch, Liverpool

Chemical Change

Sven Schroeder, Leeds

Internal/External Fields

Will Bryan, Swansea

Energy

B. Layla Mehdi, Liverpool

In-Vivo Biosciences

Angus Kirkland, RFI

AI/Data Science

Simon Maskell, Liverpool

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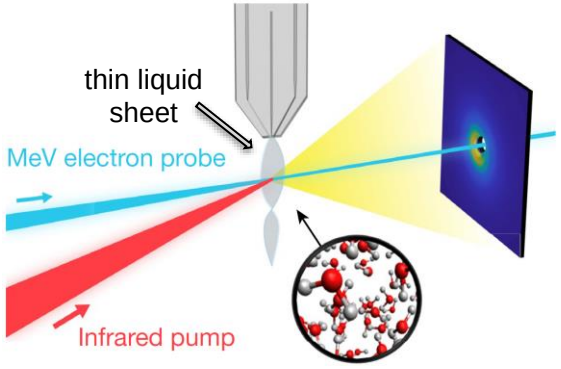
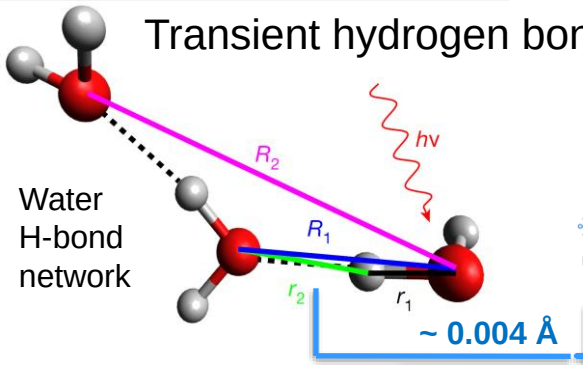
Dynamics of Chemical Change

New perspectives for control of chemical transformations – energy, healthcare, environmental, materials, biological, materials, life and medical research

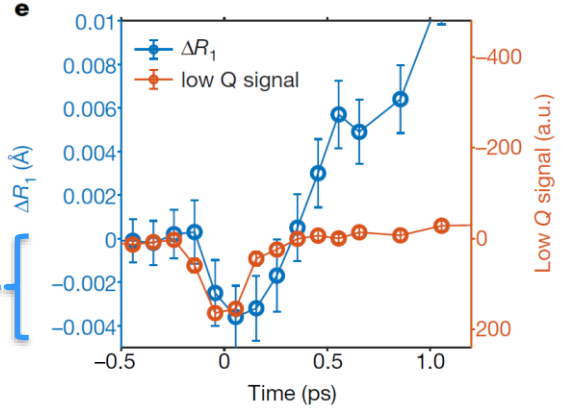
Femtosecond electron diffraction of liquids



Transient hydrogen bond strengthening during vibration



sub-ps contraction of O…H-O bond



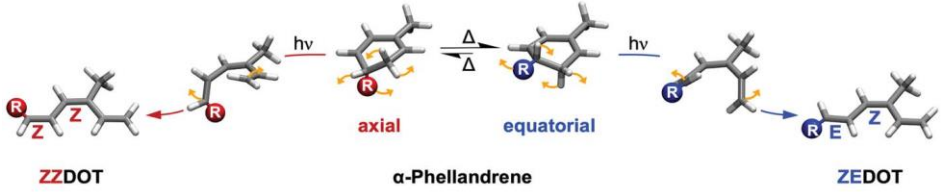
Yang et al., Nature 596 (2021) 531–535

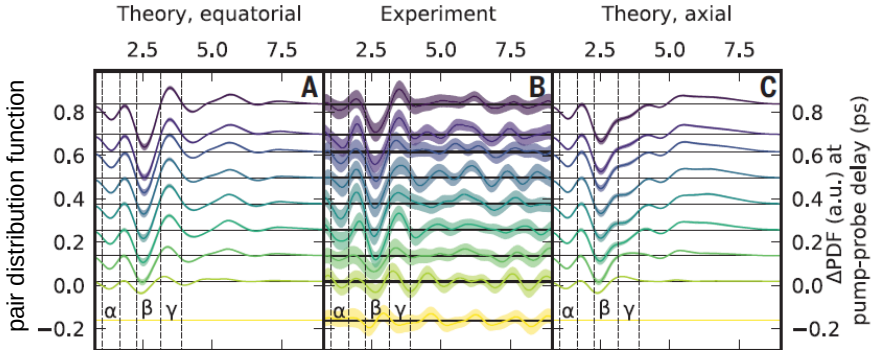
Conformer-specific photochemistry

Woodward-Hoffmann rules

Ultrafast pair distribution functions enable population analysis in conformational space

Conformational basis for photochemical branching ratios

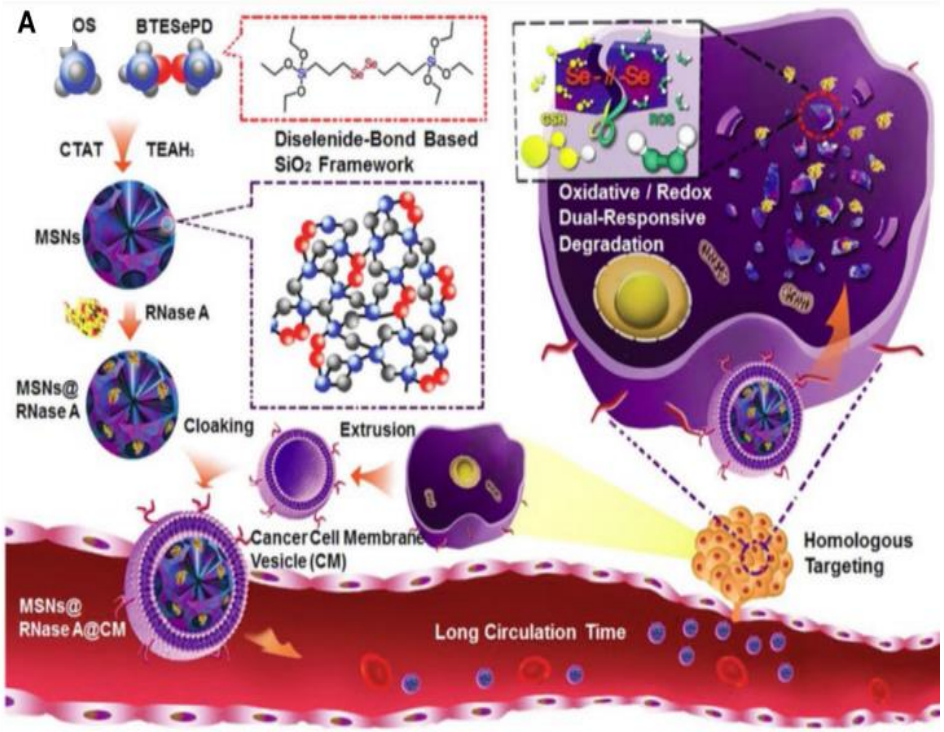




Champenois et al., Science 374 (2021) 178–182

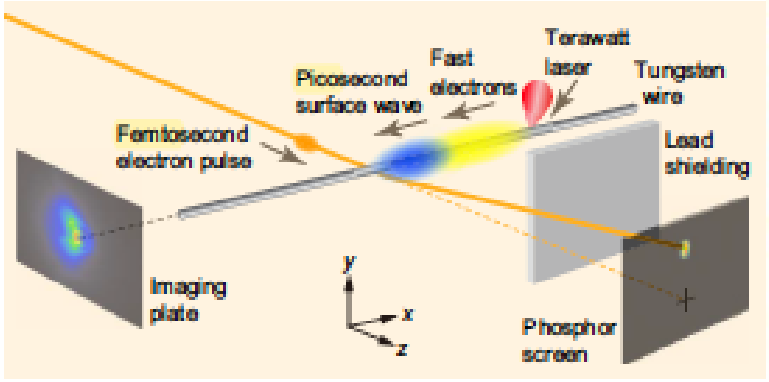
In-Vivo and Dynamical Biosciences

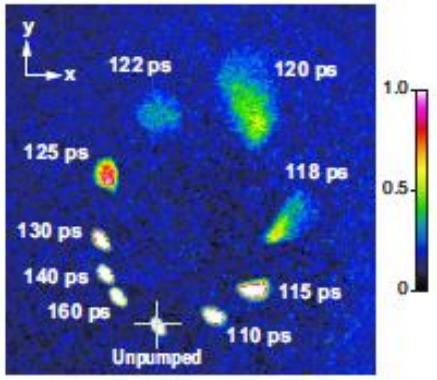
- In vitro and cryo imaging at whole cell scales – beyond medium energy tomography
- Imaging of biological structures in a cellular context
- Understanding infection and transport at high temporal and spatial resolution
- Imaging nanoparticle drug delivery and release in cells

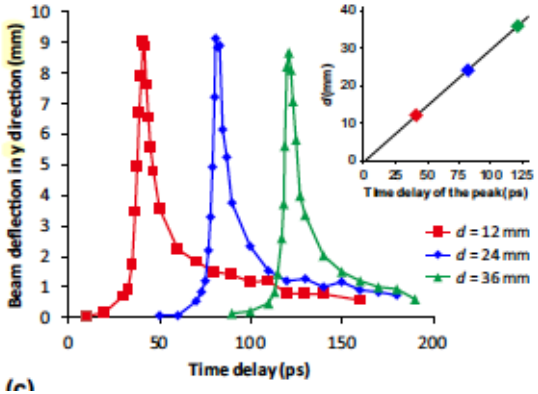


Quantum Materials & Processes

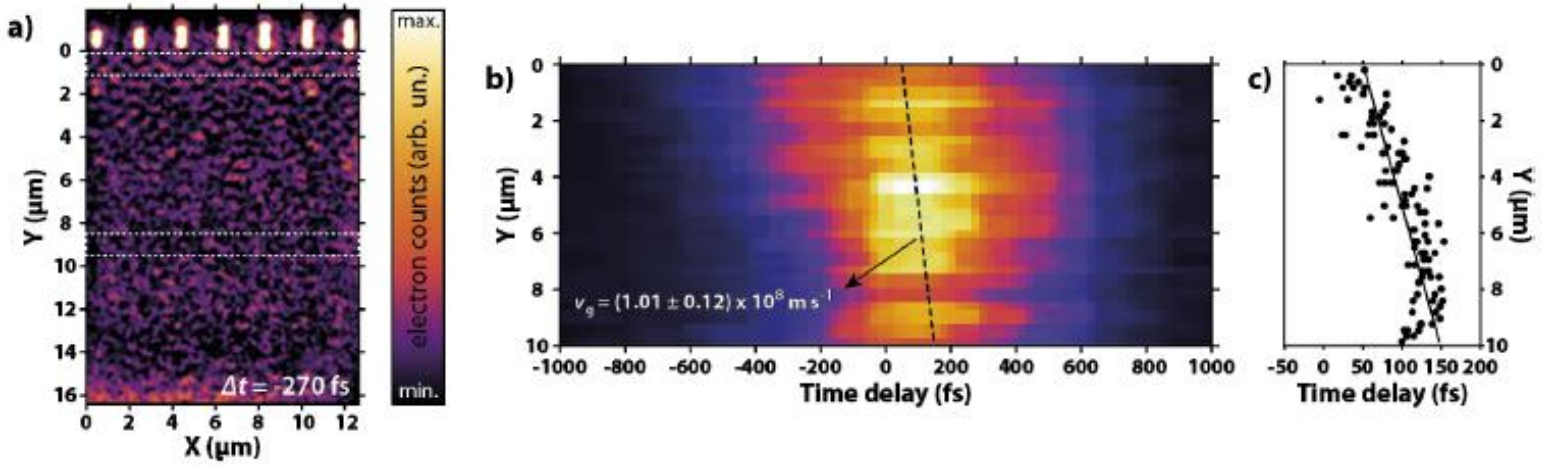
- the dynamics of electric fields







Tokita, Sakabe Sci Rep. 2015 **EB fields** ~1ps

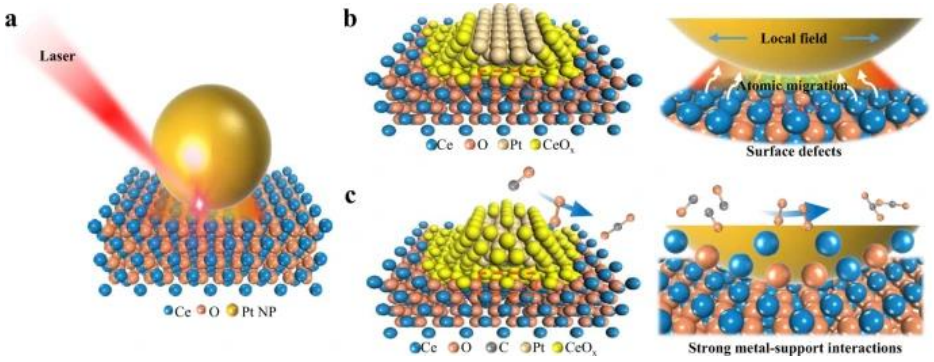


Lummen et al 2016 100fs UEM PINEM **surface plasmon polariton**

Energy Generation, Transformation & Storage

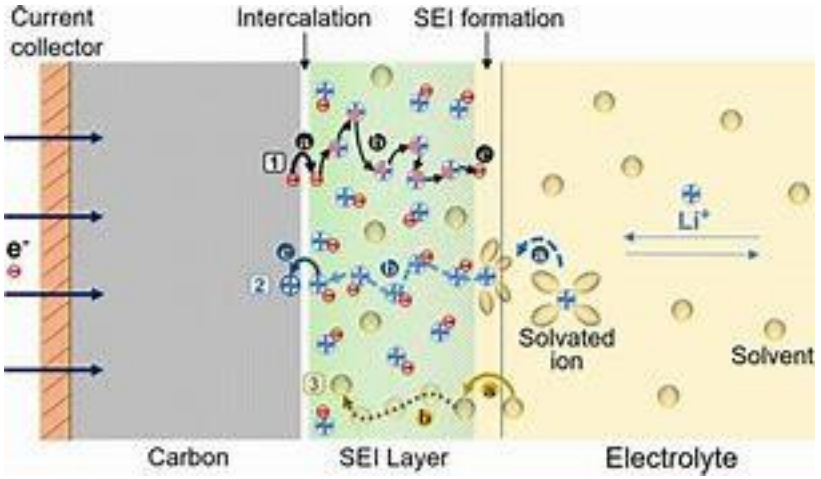
interface controlled dynamics in gases and liquids – removing the pressure gap

Heterogeneous Catalysis

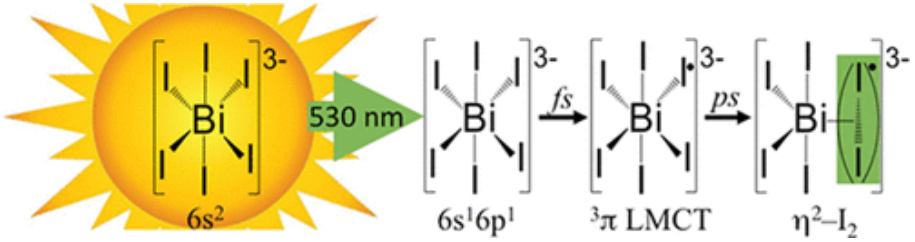


Nature Communications **volume 12**, Article number: 6665 (2021)

Next Generation Batteries



Solar Cells

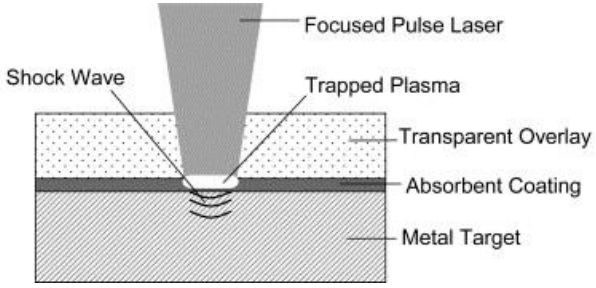


J. Phys Chem B (2022)

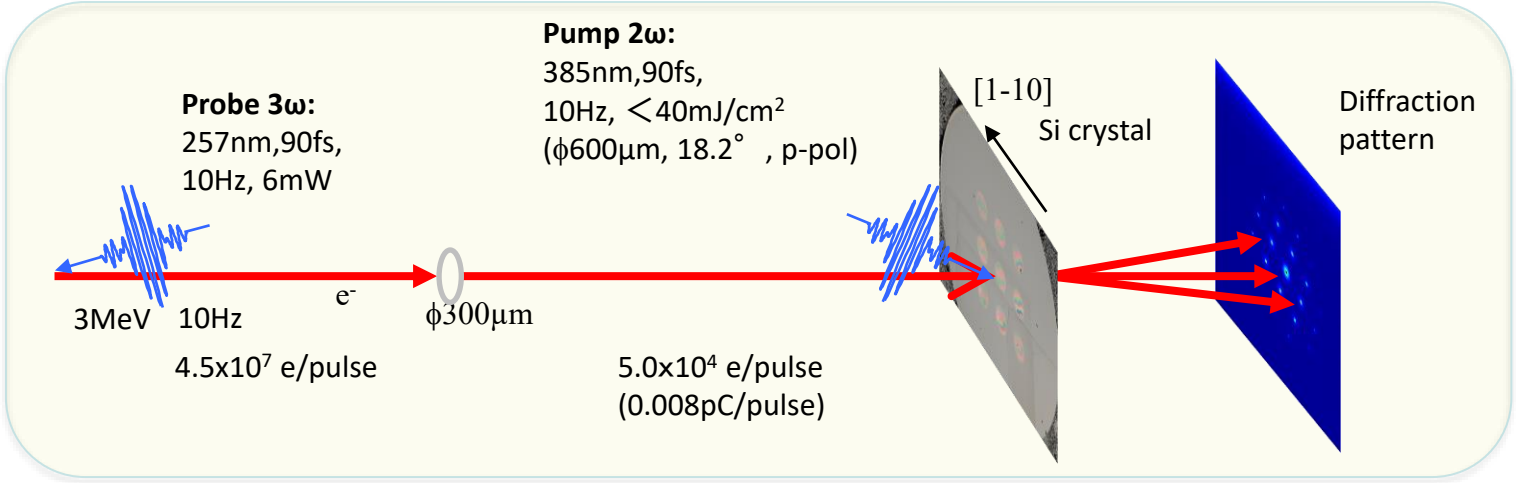
Materials in Extremes

RUEDI will provide insight into how materials and devices perform under extremes of temperature, pressure, field and environment.

- Magnetic field: Can reach **20T** as an in-plane component
- Electric field: Can reach **10^11 V/m > FEG 10^9 V/m**
- Pressure: Pulsed laser can generate a shockwave of **>100GPa**
- Temperature: Up to **ablation** of the material



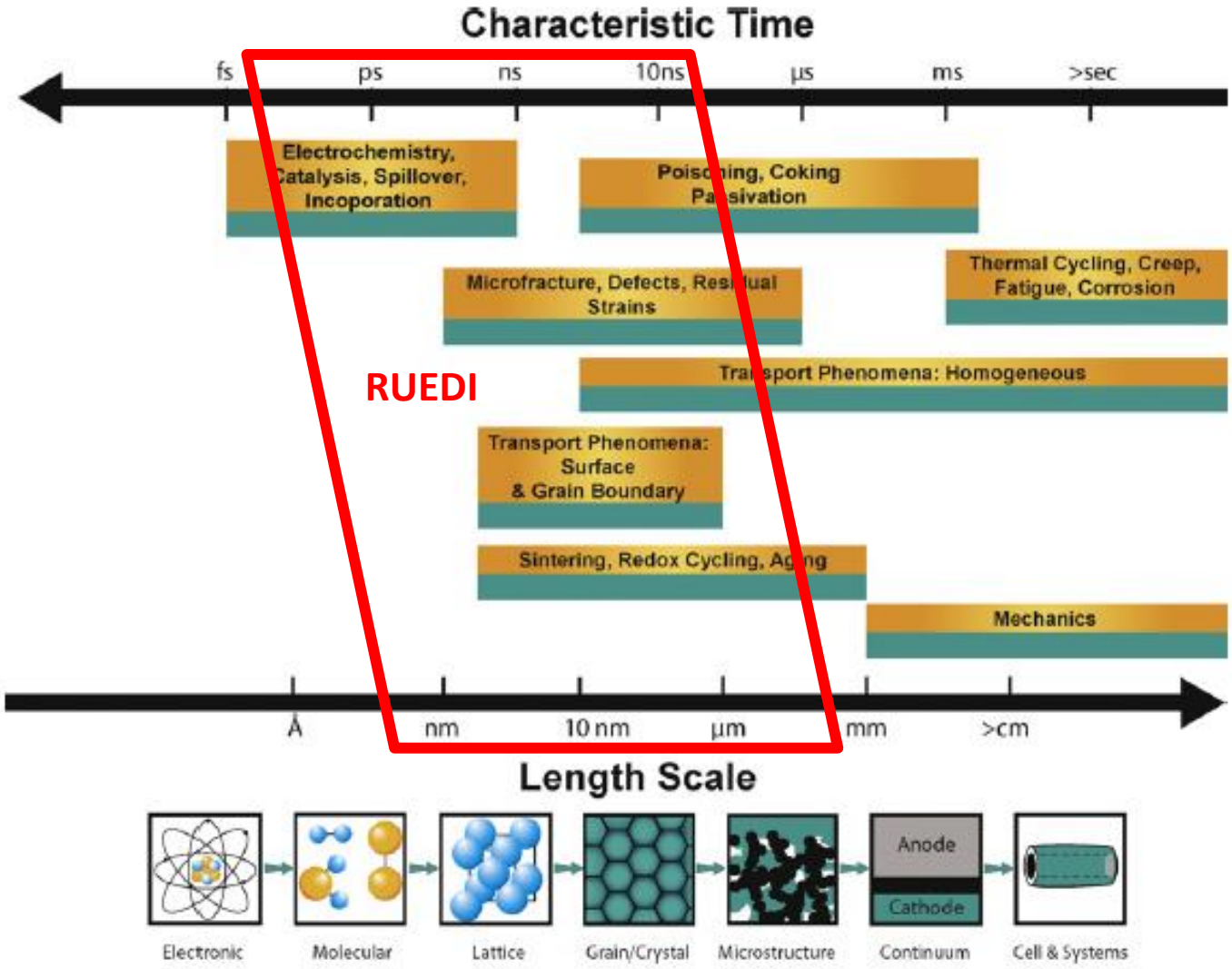
Laser Peening



Non thermal melting

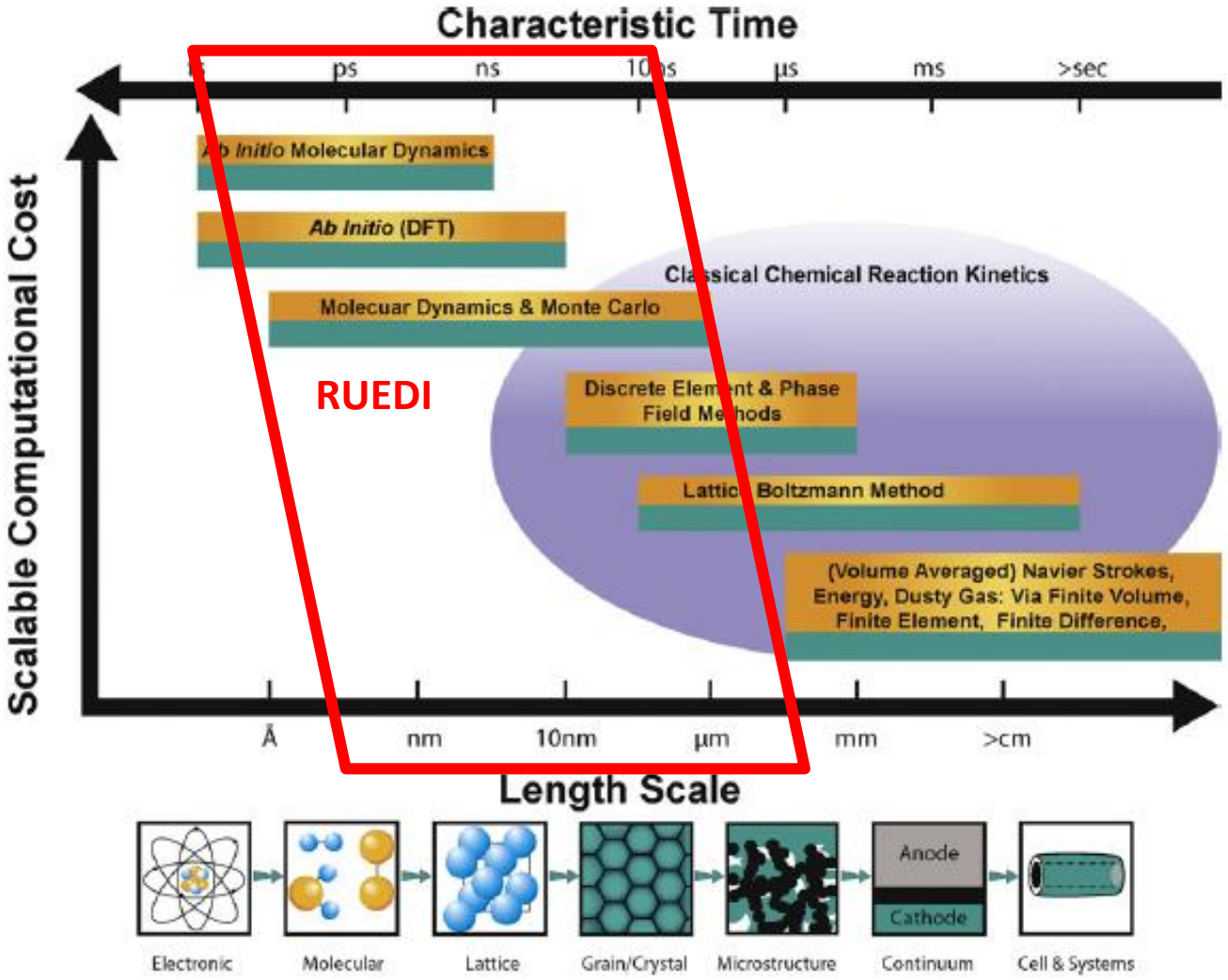
Si: UED Harb et al. PRL **100** (2008) 155504;.

Dynamic Phenomena in SOFC Materials



Grew et al.
J Power Source 2021

Beyond Classical Reaction Kinetics



Grew et al.
J Power Source 2021

Cross-Cutting: AI and Data Infrastructure

- **Digital RUEDI twin**
  - Simulate data to replicate algorithmic challenges
  - Interaction between phenomena and sensor
- **Compressive Sensing**
  - Interpolation from prior knowledge
  - Capitalise on understanding of phenomena
- **Image-free Hypothesis Testing**
  - Image is just a psychologically convenient waypoint
  - Make inferences directly using the data we have
- **Optimal Imaging of each Sample**
  - Image reconstruction as a control problem
  - Minimise photons while maximising information
- **Bayesian Optimisation & Knowledge Capture**
  - All historic data as a library of knowledge
  - Digital twin as a cheap alternative to sensing
  - Explicitly reason about when and what to image

So Why Are We Here?

We are establishing a new national facility with global impact, and to do that we want to be community driven:

- Do we have the best science themes/grand challenges?
- Do we have all the partners/collaborators/users we should?
- What experiments do you think we should do first? Why?
- What are the instrument needs for those first experiments?
- Do we need any special sample synthesis/prep methods?
- What human resources do we need to deliver the results?

CONTACT

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contact@ruedi.uk

@ruedi_uk

Relativistic Ultrafast Electron Diffraction & Imaging

world leading advances in accelerators, lenses, operando stages and detectors coupled to artificial inteligence.

RUEDI

Swansea University Prifysgol Abertawe

The Rosalind Franklin Institute

University of Toronto

UCL

University of Leeds

Imperial College London

UKRI Science and Technology Facilities Council

University of Liverpool

Next Townhall: Materials in Extremes, Cockcroft Institute, STFC Daresbury- July 21st

Discussion Sessions

Session 1: Identify Grand Challenges related to RUEDI ecosystem capabilities

Session 2: Identify Energy Sciences areas where RUEDI ecosystem can provide unique insights

Session 3: Are there specific experiments that could be defined for the RUEDI ecosystem now

In all cases feel free to nominate yourself, identify colleagues who may have interest, and make suggestions for areas to follow up with

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