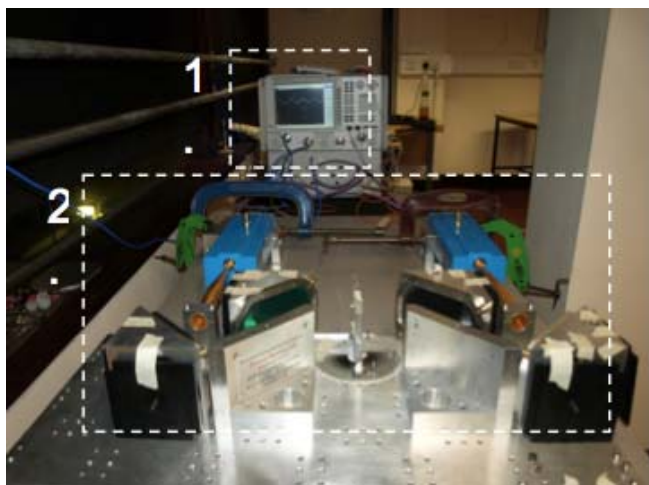


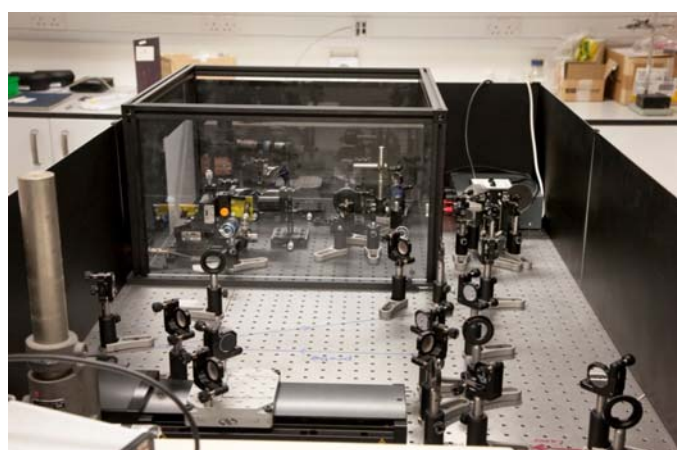
Terahertz Observational Science - Antenna & Electromagnetics Group

The Antenna & Electromagnetics Group (AEG) has a long-established expertise in electromagnetic modelling and measurement. The Group has 6 academic staff, 8 Post docs and 23 PhD students. During the last six years it has been targeting some of its expertise in experimentally developing wide band spectroscopy in the very-far infrared domain of the electromagnetic spectrum – what has latterly been dubbed by the engineering community as the terahertz (THz) region. This holds very exciting ground for new observational science, owing to the advancement of good quality sources and receivers of *coherent* radiation and the ability to control and focus the energy into solid, liquid and gaseous samples.

Through major CIF investment over the last 2 years we have developed a Terahertz facility that is unique in the UK offering both coherent vector network analyser spectroscopy up to 325GHz as well as a 0.1 to 3 THz Time-Domain Spectrometer system both housed in a purpose built vibration damped facility. The initial manpower for this activity has been part supported by the Groups EPSRC Platform grant “Antennas for healthcare and Imaging”.



The first of these systems uses a powerful state-of-the art Vector Network Analyser (VNA) shown in dashed-box 1 in the figure right, working with a Quasi-Optical (QO) circuit (dashed-box 2). The VNA is a sophisticated generator and receiver of ultra-phase-stable, coherent, finely-tunable electromagnetic radiation. It can, to date, produce as well as detect the amplitude and phase of radiation having frequencies up to 325GHz, with a capability to rise to 1THz. The QO circuit is a train of special beam-shaping mirrors that treat the sub-mm wave power as if light. The QO configuration shown here offers a focusing system that concentrates sub-mm wave power into a reaction vessel producing very high power densities at energies chosen to excite specific chemical bonds. This forms a key part of our current EPSRC “Dial a Molecule” work.



The second system is a THz TDS system based on a NPL design that has been adapted to accommodate fluid and gaseous based systems for study by either reflection or transmission configurations. The current value of our Terahertz Laboratory facility is about £700k.

We have a wide range of projects currently using the facility within Queen Mary, all of which are interdisciplinary, and the main ones are summarised below:

Selective activation of chemical bonds by active coherent THz spectrometry (Donnan):
EPSRC Chemistry Bright IDEAS Award – Dial-a-Molecule: PDRA 36 person months

‘Dial-a-Molecule’ is a current EPSRC Grand Challenge. It seeks to tackle questions of the kind: ‘How can we reliably predict how to convert one molecule into another?’ ‘How can we carry out a series of reactions sequentially?’ and ‘Can we invert modular reactions and/or reactors which can be linked to a myriad of ways to provide complex synthesis?’ It has been estimated that achieving the reality of ‘Dial-a-Molecule’ may take 20 – 40 years to realise. The adventure of this project is to investigate the very real possibility of dramatically bringing this time-frame forward to 5 years distant from now by answering these questions through activation of specific chemical bonds in any given molecule. With quasi-optical support VNAs are being used to literally dial into vibrational modes to control the reaction co-ordinate.

Coherent THz Spectroscopy for the Rapid Detection and Characterization of Bacterial Spores: (Donnan): DSTL: PDRA 12 person months:

Aims to investigate the sensitivity and selectivity for bacterial spores detection so as to meet MoD’s future requirements for pathogen detection. The work concerns testing two species of bacteria in the first instance. *Bacillus subtilis* a classic spore producing organism whose spores are commonly used to evaluate the effectiveness of autoclaves and *Bacillus cereus* a common spore producing organism causing food poisoning. Additional testing will also involve non-toxicogenic strains of *Clostridium difficile*, also a spore producing organism. Finally, for comparison we will test two classic pathogens the enteric Gram negative *Escherichia coli* and the Gram positive *Staphylococcus aureus*. Three different strains of each will be tested.

Terahertz signature of diseased cartilage (Chowdhury (SEMS)¹): PhD student (Kastriot Shala)

EPSRC *Bridging the Gap* funding for the construction of a Dispersive Fourier Transform Spectrometer that meets the specific needs of biomolecular study (in distinct contrast to traditional solid state physics). Work delivered complementary spectra of glucose and cytosine HCL to those obtained in parallel work from Time-Domain Spectroscopy conducted by us at the Time Quantum and Electromagnetics Standards Division of the NPL, Teddington. This work led to a second *Bridging the Gap* funding to begin benchmarking THz-TDS against NMR and XRD and studying protein conformation.

Exploring protein structure and dynamics using Terahertz spectrometry (Pickersgill (SBCS)² & Donnan): College funded PhD Studentship Dec 2011 to 2014

In this project correlated motions in proteins will be explored using Terahertz spectrometry. These measurements will be validated against those recorded using more traditional methods and compared to *in silico* simulations of the dynamic properties of proteins and their associated water molecules. We intend to explore structural transitions in both equilibrium and non-equilibrium systems and elucidate the role of correlated motions and fluctuations on protein function. Candidate proteins include light-responsive proteins, Aβ-peptide responsible for Alzheimer’s disease, self-assembling TPR repeat proteins and a range of enzymes involved in cobalamin biosynthesis.

Coherent, high power THz sources (Kreouzis (Physics) & Donnan): College funded PhD Studentship 2011 to 2014

Exploring hybridised integration of semiconducting polymers and conventional GaN/GaAs systems, with quasi-optics, to yield coherent, high power THz sources, started in September 2011. Being able to produce hundreds of milliwatts of THz power will make a big impact in improving THz spectroscopy which is largely used to understand enzyme-action, receptor-

¹ QM School of Engineering & Materials Science - SEMS

² QM School of Biological & Chemical Sciences -SBCS

function, patterns of DNA expression, which represent long-standing challenges in biochemistry (causes of disease) and structural biology (tracking protein folding by time-resolved spectrometry). It will also allow imaging radars operating at the lower-edge of THz spectrum. The former is of a great importance for medicine, disease-research, drug-design and beyond into synthetic biology and systems biology. The latter seeks improvement in the existing range of imaging systems to be used in non-intrusive security applications allowing detection of non-metal and composite materials.

Lagrangian mechanics applied to biological systems (Donnan): EPSRC DTA PhD studentship 2010-2013:

Lagrangian Dynamics (in either classical, semi-classical or quantum form) is being developed for mechanical interpretation of absorption spectra of bio-molecules. Motion-studies are to be performed of molecular models made up of rigid units linked, in line, by weak bending and/or rotating hinges, including viscous and capillary interactions with the solvent environment.

Our research aim is not just to provide a facility for undertaking terahertz spectroscopy but to bring to subject the rigour of calibrated measurement that can subsequently drive new predictive techniques for computational biology such as Lagrangian mechanics.