Summary

I will focus my research on three main areas, aligned with the expertise of the Antennas and Electromagnetic research group and related to the School of Engineering and Computer Science aims for teaching. The first one is to develop THz research and experimental facilities and foster collaboration with colleagues in QMUL for biomedical applications. The second direction is aimed at studying and realizing reconfigurable antennas and metamaterials at microwave and THz frequencies. Those two areas will be supported by my experience in developing bespoke numerical schemes and optimization algorithms, including the development of inovative tools based on machine learning, which constitutes the third topic that I propose to pursue.

Terahertz technologies for biomedical applications

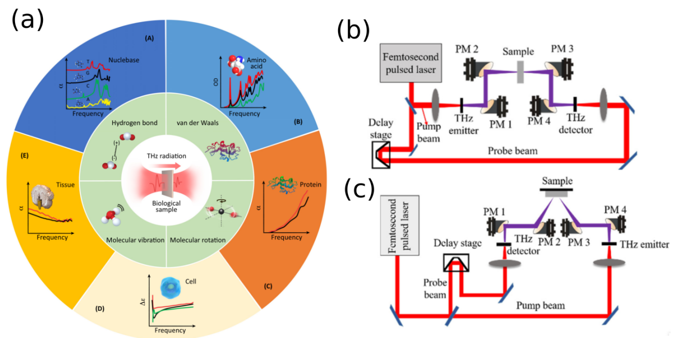

Figure 1 | (a) Biological applications of THz technologies. Typical THz-TDS imaging setup in transmission (b) and reflection (c).

Terahertz (THz) radiation generally refers to the frequency band spanning 0.1–10 THz, which lies between the microwave and infrared regions of the electromagnetic spectrum. Due to the lack of effective sources and detectors, this 'THz gap' remained unexplored until advances in physics during the 1980s. Specifically, the rapid development of modern terahertz time-domain spectroscopy (THz-TDS), has been widely utilized in applications such as materials science, astronomy, microelectronics, and biomedical science.[dhillon2017TerahertzScience2017] There has been great interest in applying THz spectroscopy to probe and characterize various biomaterials in recent decades because most low-frequency biomolecular motions lie in the same frequency range as THz radiation.[sunRecentAdvancesTerahertz2017]

I plan to foster existing collaboration between the group and colleagues at QMUL to study applications of THz science for biomedical research. Dr Akram Alomainy and Dr James Kelly, two lecturers in the Antenna and Electromagnetics group, are likely to secure a grant to invest on a new fiber optics based THz-TDS that would improve on the existing facility in term of sensitivity and spectral resolution. In addition, Professor Mira Naftaly, a Senior Research Scientist at National Physical Laboratory, has recently joined the antenna group as a visiting academic and will surely provide her expertise and invaluable insights in terahertz technologies.

Real time monitoring of proteins and biomaterial characterization: Conformational changes, which are essential for protein function, directly affect the dielectric response in the THz range (see Fig. **??**a). Due to its distinctive spectral responses to THz radiation, the dynamic hydration shell can be precisely determined by probing protein-induced fast solvation dynamics by THz spectroscopy, and predicted by molecular dynamics simulations.[sushkoTerahertzSpectralDomain2013] Innovative measurements setups, design of waveplates for efficient measurements of circular dichroism[chengQuasiOpticalSubTHzCircular2020] and parameter extraction will be explored to

help understand and monitor structural changes in biomolecules over time.
THz-TDS is an in situ non-destructive technique that has been used in QMUL to help understanding the setting mechanisms and associated dynamics of cementitious materials.[tianAtomicVibrationalOrigins2015] This collaboration with Gregory Chass in the School of Physical and Chemical Sciences would benefit from further developments to test and characterize novel biomaterials for medical and dental applications as well as natural mineralisation processes.

THz imaging: A valuable tool for exploration of materials and biological samples is the capability to do imaging, and I plan to add this feature to the experimental facilities of the antenna laboratory. In particular, THz phase imaging, an advanced imaging technology which combines the benefits of THz and commonly used phase imaging techniques, has recently received significant attention, with both pulsed and continuous-wave (CW) imaging systems.[wanTerahertzPhaseImaging2020] Pulsed THz phase imaging is a coherent measurement, which includes terahertz pulsed imaging (TPI) based on femtosecond laser and holographic imaging in the time domain, both allowing phase and amplitude information of the electric field to be recorded. CW THz phase imaging is mainly based on digital holography, interferometry and ptychography. These systems can obtain the complex amplitude by capturing diffraction patterns and applying numerical reconstruction techniques. THz imaging systems typically operate as follows (see Fig. **??**b and c): the light from pulsed femtosecond laser pumps a crystal to generate a broadband THz radiation. The scattered radiation (either in transmission or reflection mode) is mapped pixel by pixel using x-y translation of the sample or the beam in the focal plane. Off-axis parabolic mirrors are used to focus the generated THz pulse onto the sample and to collect the reflected or transmitted pulse after interaction with the sample. For biomedical imaging, systems are mostly used in a reflective geometry because the biological samples typically have high water contents and are generally strongly absorptive. I will study the feasibility of such imaging systems and apply for funding through EPSRC in close interaction with the group in order to identify the needs and most suitable technology. Another advance that I envision for biological applications is to enhance terahertz biomedical imaging by introducing exogenous contrast agents, such as gold nanoparticles, which have been shown to improve contrast.

Cells and tissue: Early studies of the origin of contrast between healthy and diseased tissue in the THz region focused on changes in water content.[yuPotentialTerahertzImaging2012] However, water content differences are not only limited to differences between healthy and diseased tissues but also the type of tissue, and that structural changes in healthy cells were responsible in part for the changes in the THz properties.[syTerahertzSpectroscopyLiver2010] Computational methods and inverse modelling are needed to interpret the EM response of biological tissues and cells. Effective media approximations have been widely used to estimate their effective permittivity. A more rigorous approach that I have successfully employed is the two scale convergence homogenization method.[guenneauHomogeniza] In comparison with analytical models such as Maxwell-Garnett or Bruggeman theories, this approach is not limited to a few canonical inclusions geometries, and can handle arbitrary topologies and media with spatially varying properties, which will help modelling accurately the interaction of tissues with THz waves, such as human skin.[wangTHzSensingHuman2021] Full wave EM simulations and high frequency[crasterHighfrequencyHomogenizationPeriodic2010] or high contrast[cherednichenkoHomogenizationSystemHighcontrast2015] homogenization techniques must be further developed, and fitting to a variety of clinical data, with the addition of inverse modelling, will help develop technology and aid better understanding of how terahertz interacts with tissues.

Enhanced detection with metamaterials and metasurfaces: Several bottlenecks exist in the development of terahertz phase imaging and detection. The lack of suitable beam shaping components to control the profile of the object illumination beam affects image quality and the lack of terahertz imaging lenses with large numerical aperture makes it difficult to collect high-frequency components and thus reduces resolution. Therefore, it is necessary to further develop high-performance terahertz sources, detectors and imaging devices. I plan to investigate the design of imaging lenses at THz frequencies, in particular using my expertise in inverse design. The fabrication will be carried out with the group's two-photon polymerization high-precision 3D printer (Nanoscribe), a state-of-the-art facility in additive manufacturing microfabrication.

Reconfigurable metamaterials and antennas

Multifunctional and reconfigurable systems are increasingly demanded for a wide range of applications in Electromagnetics and Photonics.[oliveriReconfigurableElectromagneticsMetamaterials2015] In parallel, the development of artificial media and metamaterials, allowing unprecedented control of electromagnetic (EM) waves by carefully engineered subwavelength structures, has stimulated the research interest in tunable materials. I will focus primarily on ferroelectric materials play a crucial role in microwave applications needing reconfigurability[tagantsevFerroelectricMaterialsMicrowave2018] (such as antenna beam steering, phase shifters, filters, and tunable power splitters) but plan to extend my research to other type of tuning strategies, such as phase change materials, liquid crystals, graphene or mechanically adjustable elements. Due to their inherent multi-physics and multi-scale behaviour (see Fig. **??**), ferroelectrics need improved theoretical, numerical and experimental tools as well as a proper linking of the different length scales in order to advance their understanding and guide their synthesis for use in microwave devices.

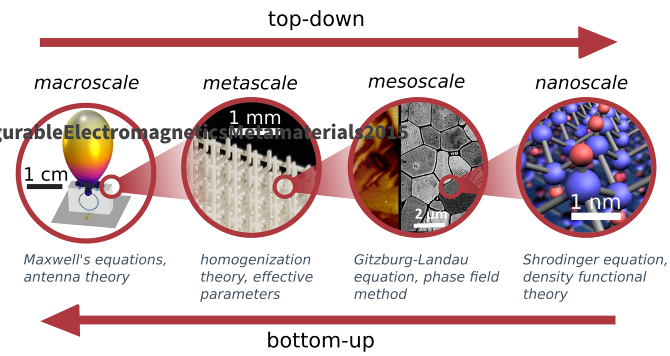

Figure 2 | Multi-scale view of ferroelectric materials and the different length scales and associated theory and modelling.

Ferroelectric metasurfaces: Structured BST film with micro-arrays have been fabricated by transfer printing in the School of Material Science at QMUL (cf. Fig. **??**). Thin BST films deposited on silicon substrate where characterized by THz-TDS and the permittivity extracted (cf. Fig. (**??**a). Transmission through the metasurface agrees well with numerical simulation with the Fourier Modal Method (FMM) where the measured permittivity of the substrate and BST were included (see Fig. **??**b). With those encouraging preliminary results, I will continue this area of research and help improve, characterize and test different BST and ferroelectric materials at THz frequencies. Geometric optimization of the microarray will be carried out to obtain functionalities such as beam steering, lensing or filtering. Change in permittivity due to an applied voltage or temperature change must be measured and will be used in further design of tunable ferroelectric metadevices. In order to extract parameters from transmission measurements, I have developed an open-source Python package[tdsxtract] with tools for pre and post processing raw experimental data, and obtain the permittivity of sample through minimization of the error between measured and analytical transmission coefficients. This will be further improved and can readily be applied to arbitrary incident angle and polarization, and would be easily extended to multilayer stacks with several layers, reflection mode operation, and anisotropic and magnetic materials.

Atomistic modelling of ferroelectrics using Density Functional Theory (DFT): *Ab initio* simulation of ferroelectic materials from their atomistic arrangement will be carried out to identify properties and new components with improved performances. Structural composition, proportions of atoms (e.g. in Barium strontium titanate (BST) $Ba_xSr_{1-x}TiO_3$ with a barium ratio of x), oxygen vacancies, can be studied by such models. In addition, the effect of external stimuli such as applied voltage, mechanical strain can be included, whilst the temperature dependence in DFT can be added *a posteriori*. The primary focus will be on the frequency dependence of permittivity and tunability, as it will affect the final design of devices in the radiofrequency and THz spectrum. Along with *in silico* new material discovery through computational material science, experimental exploration of the new ferroelectrics needs to be done to verify and inform the modeller.

Phase field modelling of ferroelectric domains: The electromechanical properties of ferroelectrics can be studied by the phase field method,[suContinuumThermodynamicsFerroelectric2007] where one considers an order parameter (usually the polarization vector) which varies continuously. Hence domain patterns with uniform polarization are separated by domain walls where the polarization switches smoothly. This intermediate mesoscale modelling is necessary and relevant as the effective properties of ceramics are often dependant of the domain arrangement and grain boundaries. Polycrystalline ferroelectrics, the effect of domain grain size, distribution, boundaries thickness, charge defects and structural inclusions, can be studied as a function of electromechanical loading, allowing to reproduce P-E loops from which one can extract the tunability and directly compare with experiments. The free energy functional used in phase field models has to be adjusted to fit the properties of single domains, and the coefficients can be obtained from DFT simulations and/or measurements.[volkerMultiscaleModelingFerroelectric2011]

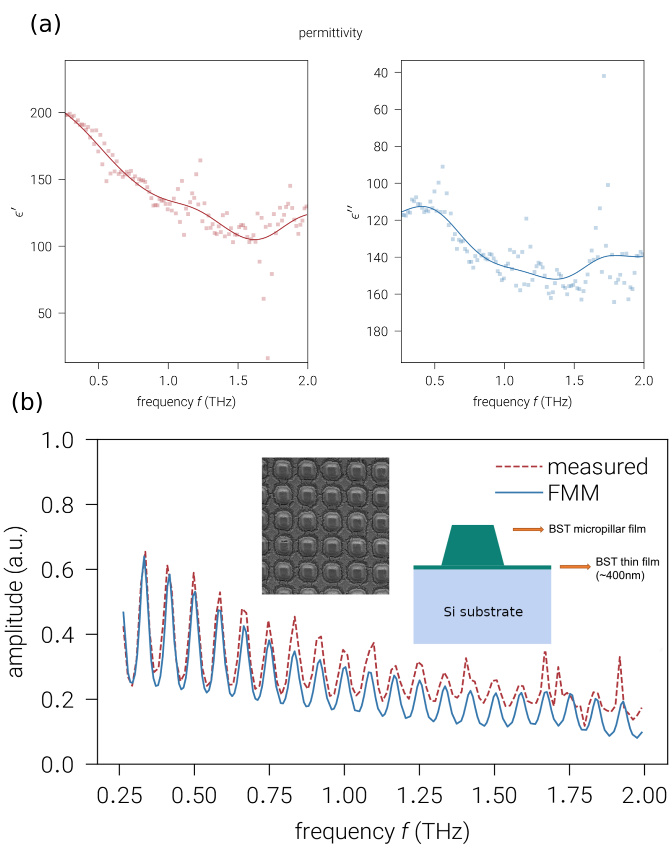

Figure 3 | BST metasurface composed of micro-pillars on thin film. (a) Extracted BST permitivity (left: real part, right: imaginary part) from THz-TDS transmission measurement of the film alone. (b) measured and simulated with the Fourier modal method (FMM) transmission through the metasurface.

Metamaterials and homogenization: I will continue the study of effective properties of ferroelectric metamaterials with subwavelength features for enhanced tunability composites.[vialEnhancedTunabilityFerroelectric2019, via] To enable the fabrication of those metaceramics and the measurement of their properties at DC, microwave and THz frequencies, I will identify relevant length scale compatible with our fabrication and measurement capabilities, including the newly acquired 3D printer with ceramic-based resins, as well as electrode layout for biasing the samples. The study of properties at the mesoscale from phase field simulations will be included in the homogenization.

Inverse design and data driven computational electromagnetism

I believe my expertise in numerical simulation and optimization algorithms would benefit the antenna group and will be a key to the success of the different research projects that I plan to undertake. I have developed bespoke open-source numerical tools employed in Electromagnetics, Photonics and antenna design that, together with commercial software, will help in designing novel devices and interpreting experimental results: (i) a versatile finite element based code[gyptis] with mesh generation, solving and post-processing complex electromagnetic problems; (ii) an implementation of the Fourier Modal Method[nannos] (also known as Rigorous Coupled Wave Analysis) with various formulations for the simulation of periodic stratified media such as frequency selective surfaces, metamaterials, photonic crystal slabs or diffraction gratings. Both codes have built-in automatic adjoint calculation capabilities that makes them suitable for gradient-based optimization.

Topology optimization:

In the past two decades, topology optimization (TO)[bendsoeTopologyOptimizationTheory2013] has become a widely used tool in computational electromagnetism[moleskyInverseDesignNanophotonics2018] and has allowed the inverse design of a broad range of devices such as invisibility cloaks illusion devices,[vialOptimizedMicrowaveIllusion2017] metasurfaces, photonic crystals and metamaterials, to name a few. Broadly speaking, density based TO is an inverse design procedure that can produce highly optimized structures serving a dedicated objective. One of its main advantage is to offer unparalleled design freedom since the material distribution is updated locally (at the pixel or voxel level) inside the domain of interest. On the other hand, fabrication constraints often limit this versatility and several auxiliary tools can be included to tackle those issues, for instance for imposing minimal length-scales or ensuring the connectivity of the resulting layout. Since the number of degrees of freedom is usually prohibitively high to obtain the gradient using naive finite differences, adjoint sensitivity analysis[jensenTopologyOptimizationNanophotonics2010] is an indispensable part of all inverse design algorithms. During my work in QMUL, I have developed general tools for inverse design of materials and devices. I plan to continue to improve those and apply them to the design of antenna devices and metamaterials, that are related with the rest of my research plans and offer my expertise to the group. One area of improvement is the inclusion of metallic parts with density based parametrization schemes, which show poor convergence because of the high contrast in material conductivities.[aageTopologyOptimizationMetallic2010] Another direction is to explore another strategy based on level-set functions that remove the unphysical intermediate material properties. Multi-objective optimization and parallelization on the school computing cluster are already implemented. This design technique allows the production of optimized parts with improved performances with often non intuitive, complex layouts, which are particularly suited for 3D printing. As an example of application, I include preliminary results on an optimized metalens for beam shaping (cf. Fig. **??**).

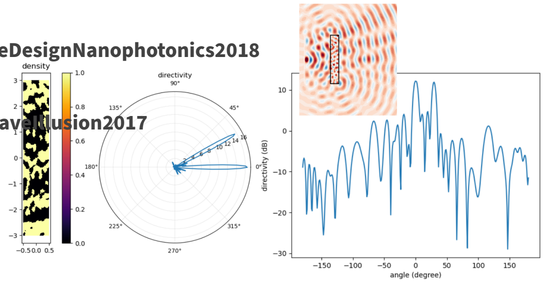

Figure 4 | Inverse design of a multi-beam lens antenna. Permittivities: material 0: $\varepsilon = 3$, material 1: $\varepsilon = 6.5$, $\tan\delta = 0.004$. Lens size = $1\lambda \times 6\lambda$. Source - lens distance = 3λ. Source – ground plane distance = $\lambda/4$. The objective is to maximize the directivity for two target angles : 0 and 30 degrees.

Machine learning:

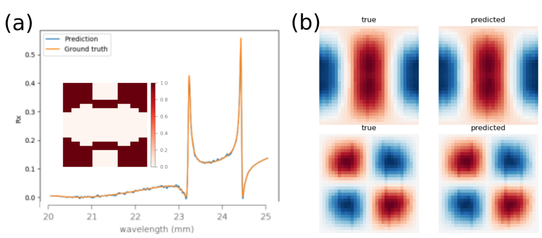

Figure 5 | Machine learning for electromagnetic design (a) Dielectric metasurface reflection spectra prediction (100 000 points in dataset, square unit cell with period=20mm made of two dielectrics with permittivity 3.0 ("0") and 4.5 ("1") and loss tangent 0.001, thickness=5mm). (b) Photonic crystal eigenmode prediction(100 000 points in dataset, input: permittivity pattern (2D, 32x32), output: 6 first eigenvalues/eigenmodes at three symmetry points of the first Brillouin zone.).

Recent advances in experimental and computational methods are increasing the quantity and complexity of generated data. Innovative approaches and tools play an important role in shaping design, characterization and optimization for the field of electromagnetism. In particular, deep learning offers an efficient means to design photonic structures,[maDeepLearningDesign2020] complementing conventional physics and rule-based methods with data-driven paradigms. My objective is to use various machine learning algorithms to predict antenna and metamaterial responses from a dataset of computer simulations. Once the neural network is trained, one obtains a fast reduced order model that can be employed to design and optimize novel EM devices very efficiently. For instance, I have developed a surrogate based global optimization code (based on a genetic algorithm), where computationally expensive objective function evaluations are partly replaced by a learned model. As an example, I have recently applied deep convolutional neural networks for predicting the reflection response from a dielectric metasurface at millimetre waves (see Fig. **??**a), which I plan to extend by training the model on both amplitude and phase data, and include different polarization of the incident wave, and use this fast model for optimization of spectral filters using a layered approach by stacking multiple permittivity patterns. Other recent results include the prediction of eigenvalues and eigenmodes of 2D photonic crystals (cf. Fig. **??**b). Eventually, once the model is trained one can predict quickly the eigenpairs at the symmetry points of the first Brillouin zone, and I plan to implement a reduced Bloch mode expansion[husseinReducedBlochMode2009] for fast band diagram and isofrequency contour calculations, so the resulting efficient simulation tool can be used for exploring and optimizing exotic physical effects such as dispersion engineering, hyperbolic media, maximized band-gap structures, exceptional and topological Photonics.