Applications are invited for a PhD studentship on:

Quantum-mechanical computational screening and design of resilient plasmonic alloys for ICT and sensing

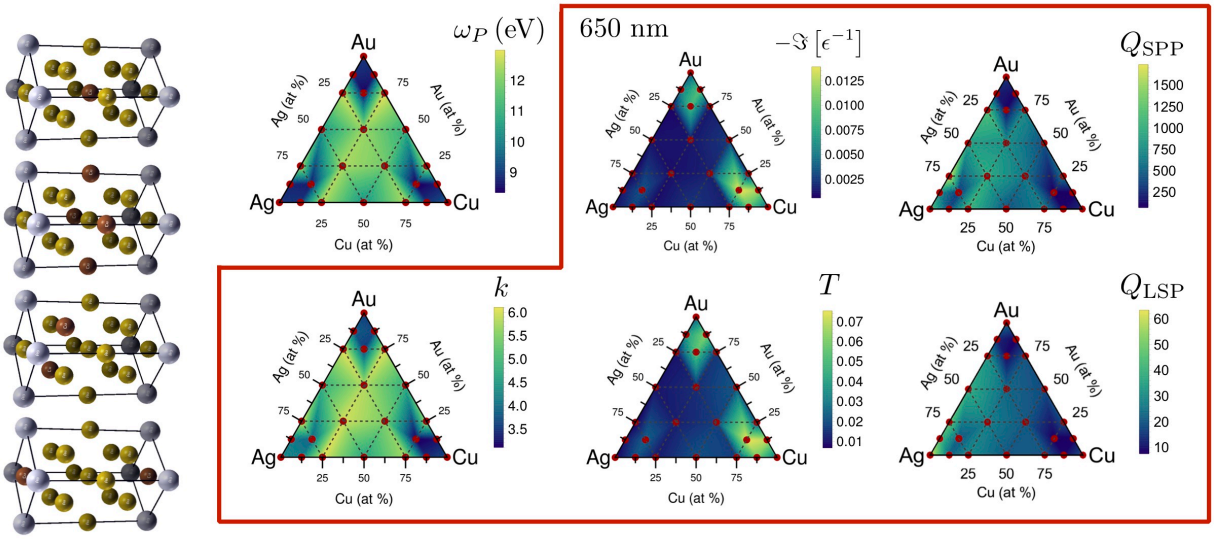
This position will be based within the **Condensed Matter Theory Group** lead by Prof. David D. O'Regan at the School of Physics and CRANN Institute, Trinity College Dublin, and form a part of the *Materials for ICT* platform within the *Advanced Materials and Bioengineering Research Centre* (AMBER).

Project Summary

The successful applicant will undertake a novel, comprehensive computational discovery program, searching for corrosion-resistant plasmonic alloys, both simple and high-entropy, focusing on optimising key figures of merit for plasmonic applications: cost, strength, weight, reliability, toxicity, manufacturability. In order to achieve this, we will together construct and showcase world-class quantum-mechanical atomistic simulation methodology (i.e., valuable software IP & consultancy spin-out opportunities) that will provide a valuable complement to ongoing experimental measurements. In particular, we will seek to identify novel stoichiometries (chemistry) and optimisation approaches that offer strategic advantages for future technology. We will also make novel use of machine learning and existing materials databases to generate new property descriptors, and combine our quantum-mechanical predictions with finite-element modeling of both plasmonic and thermal characteristics.

Background technological context

High conductivity materials, particularly metallic alloys, are ubiquitous in microprocessor, data storage and sensing technology, and are critical in high-power and high-frequency applications. The thermal conductivities and heat capacities of metals typically exceed those of semiconductors and insulators by several orders of magnitude. Thermal management is essential for gas, pressure, and temperature sensing within aerospace and terrestrial combustion technologies, e.g., in turbines, as well as for high-power lasers and LEDs. In spite of their far superior thermal performance, most high-conductivity metals cannot easily be used in high-T applications. This is due to their tendency to soften, expand and deform (creep, extrude, burnish) and to corrode, when compared to insulating ceramics. There are promising exceptions to this however: refractory metals (hard, strong, creep resistant up to high T, corrosion resistant, typically expensive, intermetallic), and the less well understood, emerging high-entropy alloys (strong, relatively light & inexpensive, randomly ordered). Innovative high-performance software development and new skills acquisition, performed while working closely with our experimentalist colleagues and our international theory partners, will enable us to significantly advance these new areas of metallurgy computationally. This will uniquely identify the PhD candidate and propel their career.



Candidate requirements
Ideal applicants will hold a 1st Class Honours Bachelor's degree in Physics, Theoretical Physics, Nanoscience, Astrophysics, Chemistry with Molecular Modelling, Materials Science, or a closely related discipline.

It is not anticipated that the candidate will be able to demonstrate significant prior experience in developing quantum-mechanical theory, in software development, or high-performance computing cluster use. However, a clear interest in these areas, and lots of enthusiasm for spending time working very deeply on challenging intellectual problems with the aim to bettering their own skill-set, problem solving and scientific communication abilities, and for benefitting wider society, will be required. Some prior experience in basic coding or shell scripting, or a prior research project involving that, may be beneficial. This is an applied quantum mechanics project combining electronic structure theory, quantum and classical thermal modeling, and finite-element electromagnetics. A candidate who enjoyed undergraduate topics such as electromagnetic theory, atomic physics, condensed matter, linear algebra and multivariate calculus is likely to find this project extremely rewarding. It is envisaged that the candidate will be willing to take an appropriate secondment at a research group overseas during their studies. The candidate should be willing and enthusiastic to represent the AMBER platform and Group internationally e.g., at conferences, workshops, training schools and in collaborative visits.

A broad range of very relevant, highly-marketable skills and competences are likely to be developed by the successful PhD candate. Upon completion, they should be able to demonstrate advanced data analysis and graphical skills; excellent oral presentation skills (an enthusiasm for public outreach and engaging with junior students is welcome); the ability to confidently and independently use high-performance computing resources; the initiative and discipline to manage their own time and project tasks, and to understand the needs of diverse collaborators and potential research sponsors. Such competences are prized across diverse work environments.

The PhD canidate will work closely with other members of the multidisciplinary project team. Open, routine collaboration with other groups within the ICT platform and with overseas partners will be required, together with frequent reporting and performance management. Excellent written and oral communication skills, as well as a collaborative, collegial, and resourceful disposition are essential. Diversity in all its forms is highly valued by the Condensed Matter Theory Group, and we strive to foster a supportive, friendly, productive work ethos.

How to apply:
CVs with the names and addresses of three referees, together with one or two representative examples of the candidate's written work (for example an undergraduate research project report), should be submitted to:

Prof. David D. O'Regan <David.O.Regan@tcd.ie>
School of Physics, Trinity College Dublin

Web: http://physics.tcd.ie/condensed-matter-theory-group
Twitter: OReganGroupTCD

Informal enquiries are very welcome. Positions will remain opened until filled and the preferred start date is September 2nd 2019. Only short-listed applications will be acknowledged due to time constraints.

This PhD studentship is funded by the SFI research centre AMBER.

The AMBER research centre, as a community of researchers, welcomes its responsibility to provide equal opportunities for all. We are actively seeking diversity in our research teams and particularly encourage applications from underrepresented groups.