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Theory and simulation of semiconductor nanowire quantum-confined heterostructures

Applications are invited for a four-year Ph.D. studentship in theoretical and computational condensed matter physics at the School of Physics, University College Cork (UCC), under the supervision of Dr. Christopher Broderick. The studentship is funded by a recently awarded Royal Society-Science Foundation Ireland University Research Fellowship, includes a stipend of €22,000 per annum, and pays full tuition fees.

The project centres on the theory and in silico design of heterostructured semiconductor nanowires (NWs), to identify and optimise targeted optical and electrical properties underpinning potential applications spanning a range of classical and quantum photonic and electronic device technologies.

Two classes of NW heterostructures are of interest: (i) radial “core-shell” heterostructures in which the material composition is varied in the direction perpendicular to the NW axis, especially core-shell NWs based on direct-gap group-IV alloys including GeSn, and (ii) axial “polytype” heterostructures formed by alternating the crystal structure of a given group-IV or III-V material between its stable cubic (diamond or zinc blende) phase and its metastable hexagonal (lonsdaleite or wurtzite) phase, especially polytype NWs based on direct-gap lonsdaleite group-IV SiGe alloys and on direct-gap wurtzite III-P alloys. NW heterostructures of type (i) are of interest for the development of efficient infrared-wavelength light emitters for integrated Si photonics. NW heterostructures of type (ii) are of interest for the development of novel Si-compatible transistor architectures, for applications in integrated Si photonics, and to address the so-called “green-gap” for visible-wavelength emitters in solid-state lighting and display technologies.

Developing quantitative understanding of the properties and performance of photonic and electronic devices based on these nanostructures mandates, in the first instance, developing predictive atomistic quantum mechanical calculations of the NW properties. Beginning from first principles calculations based on density functional theory, the student will develop transferable interatomic potentials and model Hamiltonians that allow to accurately describe the fundamental properties of both the cubic and hexagonal phases of group-IV and III-V semiconductor materials. These models will enable accurate large-scale atomistic electronic structure calculations for NW heterostructures, providing input to develop predictive calculations of key properties relevant to device applications (e.g. radiative and non-radiative carrier recombination rates for applications in NW-based photonic devices). The results of these calculations will then guide in silico optimisation of candidate heterostructures for targeted device applications.

The project will encompass a combination of model development and parametrisation, software development, and high-performance computing. The outcome of the project will constitute a new state-of-the-art in the understanding of the fundamental properties of heterostructured semiconductor NWs, and provide guidance to material growers and device engineers working on novel material concepts to deliver enhanced performance and new capabilities in next-generation semiconductor devices.

The project will empower the student to develop a range of analytical, computational and transferable skills which, at the conclusion of the Ph.D., will place them in a competitive position to undertake postdoctoral research or to obtain a high-value position in industry.

Additional responsibilities:

- Demonstrate commitment to, and engage in, technical and professional development training
- Publish research results in leading international journals
- Present research results at leading international conferences and workshops
- Attend and participate actively in regular supervisory and research group meetings
- Engage with project collaborators
- Contribute positively to the academic culture of the School of Physics
- Contribute to the mentoring and supervision of undergraduate project students and research interns
- Participate in education and public engagement activities in line with institutional policy
- Carry out any additional duties that may reasonably be required within the scope of a Ph.D. studentship

Essential criteria:

- Recent completion, or expected near-term completion, of a B.Sc. or M.Sc. degree in physics or a closely-related discipline, having achieved an overall grade of first or upper-second class honours or equivalent: https://ucc.ie/en/study/comparison/
- Coursework including condensed matter physics, computational physics and/or semiconductor device physics
- Demonstrable experience working with a programming or scripting language (e.g. C/C++, Python)
- Good interpersonal and communication skills, and an ability to work in a collaborative environment

Desirable criteria:

- Research experience related to the theory and simulation of semiconductor materials and/or devices
- An evidenced interest in, and aptitude for, scientific computing and software development
- Commitment to open science, including open-access publication and dissemination of research data/software

To be considered for this position, applicants should submit:

- A cover letter outlining their interest in, and any experience relevant to, the research project (max. 1 page),
- An up to date CV including details of relevant training, skills and experience, in addition to details of undergraduate courses taken, grades achieved and projected overall degree grade (max. 2 pages), and
- A minimum of one academic reference letter (e.g. from a research project or internship supervisor)

via email to Dr. Christopher Broderick (email: christopher.broderick@ucc.ie).

The closing date for receipt of applications is Friday, April 26th, 2024.

Informal enquiries may be directed, in confidence, to Dr. Christopher Broderick (via the email address specified above).

Applicants whose first language is not English must additionally provide evidence of English language proficiency, in line with UCC regulations: https://ucc.ie/en/study/comparison/english/postgraduate/. English language certificates should be valid at the time of application (usually less than 2 years old).

Appointment to this position is subject to approval by UCC, in line with the terms of the Employment Control Framework for the Higher Education Sector. Vetting by An Garda Síochána and/or an international police clearance check may form part of the selection process. UCC may, at its discretion, undertake to make additional appointments from this competition following the conclusion of the selection process. UCC is an equal opportunities employer.