



Role profile

Job title	Research Associate/Fellow in Modelling Electronic and Quantum Properties of 2D Semiconductors	Job family and level	Research &Teaching Level 4
School/ Department	School of Chemistry	Location	University Park Campus

Purpose of role

The purpose of this role is to conduct computational studies of electronic transport and quantum phenomena in 2D semiconductor materials (2DSEM) and spin-qubits; work in close collaboration with partners in academia and industry to address challenges in the science and technology of atomically thin semiconductor for low-energy-consumption electronics; aid the design of 2D Dirac-source FET.

	Main responsibilities (Primary accountabilities and responsibilities expected to fulfil the role)	% time per year
1	Research activities: Use scientific literature and previous research experience to contribute to the research objectives of deeper understanding the emergent properties of 2D semiconductor materials and aid the development of new 2DSEM-based device architectures.	60%
2	Prepare high quality papers for publication in leading peer-reviewed journals.	20%
3	Give presentations internally at group meetings and externally at conferences	5%
4.	Identify and develop opportunities for research grant funding proposals.	5%
5.	Provide support, guidance, and co-supervision to undergraduate and/or postgraduate research students	5%
6.	Any other duties appropriate to the grade and role of the post holder as necessary.	5%

Person specification

	Essential	Desirable
Skills	<ul style="list-style-type: none"> Strong skills in computer programming in a chemical context; experience in programming using one or more of the following languages: C, C++, Fortran 77/90/03, Python In-depth knowledge of many-body Green's function theory to study local perturbations in solids In-depth knowledge of and experience in developing hybrid electronic structure methods Strong mathematical background 	<ul style="list-style-type: none"> Ability to use a range of software packages such as ORCA, QChem, CP2K and/ or GPAW.
Knowledge and experience	<ul style="list-style-type: none"> Track record in electronic structure calculations of transport and quantum properties Good communication skills, both orally and in written English, suitable for the preparation of scientific publications in world-class journals and presentation of research at international conferences Well organised and self-motivated with the ability to manage the day-to-day running of a research project. 	<ul style="list-style-type: none"> High quality research publications in international peer-reviewed journals. Experience in applying quantum chemical approaches to investigate electronic transport and quantum phenomena in 2D semiconductor materials and spin-qubits Working on a collaborative project
Qualifications, certification and training (relevant to role)	<ul style="list-style-type: none"> PhD (or near completion) in Computational Chemistry or related area. 	<ul style="list-style-type: none"> Established reputation for research in computational chemistry.

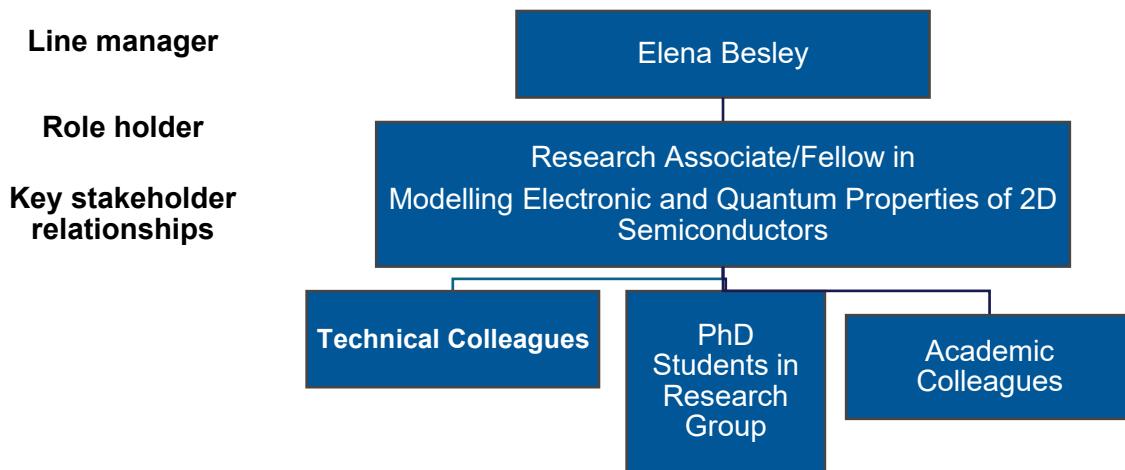


Expectations and behaviours

The University has developed a clear set of core expectations and behaviours that our people should be demonstrating in their work, and as ambassadors of the University's strategy, vision and values. The following are essential to the role:

Valuing people	Is friendly, engaging and receptive, putting others at ease. Actively listens to others and goes out of way to ensure people feel valued, developed and supported.
Taking ownership	Is clear on what needs to be done encouraging others to take ownership. Takes action when required, being mindful of important aspects such as Health & Safety, Equality, Diversity & Inclusion, and other considerations.
Forward thinking	Drives the development, sharing and implementation of new ideas and improvements to support strategic objectives. Engages others in the improvement process.
Professional pride	Is professional in approach and style, setting an example to others; strives to demonstrate excellence through development of self, others and effective working practices.
Always inclusive	Builds effective working relationships, recognising and including the contribution of others; promotes inclusion and inclusive practices within own work area.

Key relationships with others



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