Department of Chemistry

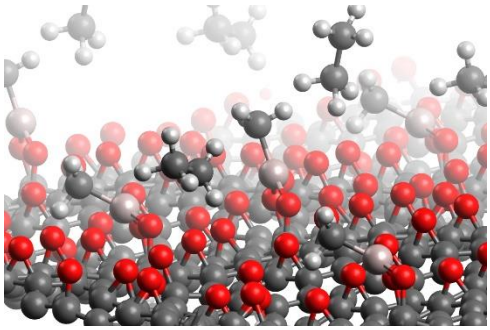
WARWICK
THE UNIVERSITY OF WARWICK

PhD Studentship in AI-supported Computational Chemistry of Materials

Project: Atomistic Simulations of Surface Chemistry underpinning the Atomic-Scale Processing of Materials for AI-driven Nanoelectronics Applications
Supervisor: Dr. Bora Karasulu (Assistant Professor in Computational Chemistry, Chemistry Department)
Closing date: Open until filled
Start Date: As soon as possible

A fully-funded 3-year PhD studentship is now available in the Karasulu Lab at Warwick.

Project description:



Atomic layer deposition (ALD) and atomic layer etching (ALE) are crucial technologies in semiconductor processing, especially as nanoelectronics devices become smaller and more complex. ALD/ALE offer sustainable processing by using minimal materials and chemicals due to self-limiting reactions. Their reproducibility across different runs, tools, and facilities makes them ideal for predictive AI models, applicable in various stages of process development, monitoring, and control.

The progression of AI-driven process development and material synthesis relies on comprehensive training data accessible via databases. Supported by two major semiconductor industry players (**Intel** and **Merck**), this research programme aims to expand our crowd-sourced databases containing ALD and ALE processes to unlock AI-compatible atomic-level processing approaches. It also seeks to explore novel avenues for AI-driven process development, material design, and autonomous experimentation. The ultimate objective is to decrease material consumption and enhance sustainability in semiconductor fabrication processes.

The research program unites three research groups from the University of Warwick, Eindhoven University of Technology (**TU/e**, Netherlands), and the L3S Research Centre at Leibniz University of Hannover (**L3S**, Germany). It focuses on three distinct perspectives: (**WP1**) Experimental process development aims to populate the databases with experimental data and integrate data from predictive AI models into future R&D labs and production fabs; (**WP2**) Materials modelling seeks to populate databases with theoretical data obtained through surface chemistry modelling, integrating AI-predicted data and materials into computational workflows.; (**WP3**) Data science emphasises knowledge input and extraction from databases and literature through the development of AI Large Language Models (LLMs).

As an essential component of our research programme (**WP2**), our group conducts multi-scale modelling of the chemical processes occurring at material surfaces within semiconductors, which underpin the related ALD and ALE processes. Additionally, we engage in high-throughput discovery of coating materials and the in-silico characterisation of their various properties, facilitating direct comparison with

experiments performed by the project partners. Consequently, the PhD candidate in our group will utilise a wide range of *state-of-the-art* computational modelling methods, including Density Functional Theory (DFT) and machine-learning interatomic potentials (MLIPs), while also contributing to their development. These tasks necessitate calculations that are run on local and national-scale high-performance computing (HPC) facilities. Our research is closely coordinated with the leading experimentalists from TU/e and computer scientists from L3S. The PhD student will have ample opportunities to interact with these collaborators and fellow PhD-student peers through regular online and in-person meetings. Additionally, the postholder will participate in monthly update calls with the **Intel-Merck consortium**.

Selected Publications: [1] *J. Mater. Chem. A*, 2024, **[2]** *Adv. Mater.,* 2023, **[3]** *J. Am. Chem. Soc.,* 2022**, [4]** *Carbon*, 2022 **[5]** *Phys. Rev. Mater.*, 2020; **[6]** *J. Am. Chem. Soc.,* 2020; **[7]** *ACS Nano*, 2017; ALD and ALE databases: https://www.atomiclimits.com/aledatabase/ *Copies are available upon request; also see my Scholar profile.

Qualifications / Requirements: Candidates should hold an honours degree (minimum UK 2.1 or equivalent) in chemistry, physics, material sciences or other related fields. While prior experience in electronic structure theory, condensed matter theory, data analysis using Bash/Python/C++ scripts, software development (e.g., Python, C++, or similar), and familiarity with Linux and high-performance computing (HPC) environments is advantageous, it is not mandatory. Similarly, experience in modelling solid-state materials and/or surface chemistry is a plus. The successful applicant will receive an initial training in molecular modelling, data sampling, and analytics methods. We seek enthusiastic team players eager to learn, innovate, and contribute to an exciting research field!

Funding availability: Fully funded for Home, EU and international applicants; only full- time employment. The studentship is funded through the AI-Aware Pathways to Sustainable Semiconductor Process and Manufacturing Technologies (AWASES) programme grant provided by the **Intel-Merck Consortium** and it provides funding for 3 years, covering the maintenance and Home tuition fees, and a budget for the travel and training expenses along with a research support. The tax-free stipend is at the standard research council rates (currently at £18,622 p.a) with annual increments, see here). The student will not have any mandatory course load, however they will have access to the rich PhD-level training programme offered by the Chemistry PG School and EPSRC HetSys CDT programme. Some funding opportunities are available for overseas students (see here), contact us for information.

How to apply: When applying for this post online, please attach the following documents: (1) **Your CV** including your most up to date qualifications and a summary of your education to date along with the contact details for **two academic referees**, and **list of publications** (if any)and (2) a **supporting (personal) statement** (max 2 pages) outlining your interest in pursuing a PhD within the research area of the studentship, particularly in the advertised project, and your suitability for the role. Referees will be contacted during the interview stage, so please notify them in advance. Shortlisted candidates will be **interviewed at the earliest opportunity**. Please direct informal enquiries and requests for further information to Dr. Bora Karasulu (bora.karasulu@warwick.ac.uk).

For information regarding the application process, see https://warwick.ac.uk/study/postgraduate/apply/research/. For further details about the research group, see https://warwick.ac.uk/fac/sci/chemistry/staff/borakarasulu/; and for Warwick Chemistry postgraduate courses, see this page.