EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems

HetSys

Launch Event

9 – 10 September 2019

University of Warwick

Programme

Location: Room MS B3.03, Mathematics Department, Zeeman Building, University of Warwick, Coventry, UK

Monday 9th September 2019

10:30 Registration and tea/coffee

11:00 Welcome on behalf of University of Warwick
Pam Thomas, Pro-Vice-Chancellor (Research)

11:15 Overview of HetSys – overall scope, training and engagement opportunities

11:45 Description of HetSys research themes, 2019 HetSys PhD projects, supervisors and students

12:30 HetSys 2020 PhD projects co-creation including overview of initial suggestions

13:00 Lunch

14:00 Identify groups to develop 2020 HetSys PhD projects

14:30 Highlight Talk 1 – *Ab initio simulation of finite-temperature phase stabilities: Concepts and applications*
Tilmann Hickel, Max-Planck-Institut für Eisenforschung

15:00 Highlight Talk 2 – *Multiscale modeling of solid/liquid interfaces*
Paola Carbone, University of Manchester

15:30 Tea/coffee

16:00 Poster session – expertise marketplace for HetSys staff, colleagues, partners

17:00 Wine and whiteboard session – groups develop PhD project outlines

19:00 Dinner, Radcliffe Restaurant, University of Warwick campus

Tuesday 10th September 2019

9:30 Highlight talk 3 – *Mathematics and molecular dynamics*
Tony Lelièvre, CERMICS, Ecole des Ponts, Paris

10:00 Highlight talk 4 – *Microscopy – where modelling meets reality*
Richard Beanland, Microscopy Group (Physics) University of Warwick

10:30 Tea/coffee

11:00 Groups prepare summary presentations of 2020 PhD projects*

11:30 Group representatives present to rest of participants (5-10 mins each)

12:30 Lunch

14:00 Highlight talk 5 – *Molecular simulations you can trust and reproduce: The OpenKIM framework*
Ryan Elliott, OpenKIM project, University of Minnesota

14:30 Summary. List of proposed PhD projects for 2020 including those resulting from this launch event. Supporting activities for developing partnerships and ongoing project co-creation (e.g. study groups, internships, undergraduate summer projects)

15:00 Tea and cakes

16:00 Finish

* From 11:00-12:30 on Tuesday there will be a parallel activity for new HetSys students

Travel to the University of Warwick

The HetSys Launch Event will be held in Room MS B3.03 of the Zeeman Building (Mathematics and Statistics), on the University of Warwick Campus.

Postcode for SatNav: CV4 7AL

Interactive Campus Map: https://warwick.ac.uk/about/visiting/maps/interactive/

Wi-Fi

Warwick Guest

Conference attendees, short term guests and visitors to the University of Warwick have free access to a centrally managed wireless network service. Connect to the "**Warwick Guest**" network.

eduroam

For those visiting from another academic institution that participates in the eduroam service, the eduroam wireless network service is available across the campus at Warwick.

https://warwick.ac.uk/services/its/servicessupport/networkservices/wifi/

Dinner

Dinner is on Monday at 19:00 in the Radcliffe Restaurant on campus.

Parking

If you have reserved visitor parking, it will be in Car Park 15.

Accommodation

Best Western Plus Windmill Village Hotel, Golf Club & Spa

Birmingham Road, Allesley, Coventry, CV5 9AL

There will be a shuttle bus between the hotel and campus.

Shuttle bus times

Monday 09/09/19
10:00 pickup at hotel, to arrive at the Zeeman Building at 10:15

21:15 pick up at Radcliffe to return to the hotel
21:45 second pickup at Radcliffe to return to the hotel

Tuesday 10/09/19
9:00 pickup at hotel, to arrive at the Zeeman Building at 9:15. Please note that there will be one shuttle bus and one taxi. The shuttle bus seats 16 and the taxi seats 5.

Abstracts

Monday 14:30 Highlight Talk 1

Ab initio simulation of finite-temperature phase stabilities: Concepts and applications

T. Hickel, J. Janssen, H. Sözen, F. Körmann, J. Neugebauer

The performance of heterogeneous metallic alloys is determined by their microstructure, containing a combination of different phases and/or extended defects such as interfaces and stacking faults. Their stability usually depends on the chemical composition and the temperature of the material. While established ab initio methods are very well suited to cover the first aspect, the finite temperature phase stabilities are rarely explored. This is connected to the fact that density functional theory is designed to provide ground state properties. The extension to finite temperatures requires the consideration of vibrational, electronic, magnetic and configurational entropy contributions, for which complex simulation protocols are required. We have created a Python based framework called pyiron, which provides an integrated development environment for such protocols and allows one to upscale them for high-throughput simulations on large computer clusters. After explaining the underlying methodological concepts, we use the example of the hard-magnetic material system Ce-Fe-Ti to demonstrate the materials scientific consequences. Since the promising magnetic phase CeFe11Ti thermodynamically competes with various Laves phases, the partitioning of several additional elements and their impact on the relative phase stabilities have been considered. The insights obtained demonstrate how the screening of a large set of transition metals in the quaternary hard magnetic materials can be performed most efficiently and which alloying elements improve the stability of CeFe11Ti most substantially.

Monday 15:00 Highlight Talk 2

Multiscale modeling of solid/liquid interfaces

Paola Carbone

Solid/liquid interfaces are ubiquitous from devices to composite materials and are deemed to predict and control the device efficiency and the material properties.

In this talk we will present two different multiscale approaches to predict the structure and dynamics of two different solid/liquid interfaces. In the first example we will focus on polymer/surface interfaces and present an easy and fast way to develop the cross-terms (i.e. solid/liquid) for chemically-specific coarse-grained potential terms. The newly developed models predict the same interfacial structure as obtained from atomistic simulations but allows the simulations of large entangled melt.

In the second example, we will present a new procedure to develop ions/graphene interactions for electrolyte solutions in contact with graphitic surfaces. Despite producing a classical model, the new procedure can reproduce the experimental ions adsorption energies which are dominated by the polarization of the surface as the ions approaches.

The aim of these multiscale techniques is to balance the need to retain important chemical details allowing long simulations and ultimately to identify design rules to predict the liquid/surface adhesion properties as a function of surface roughness and liquid compositions.

Tuesday 9:30 Highlight Talk 3

Mathematics and molecular dynamics

Tony Lelièvre

Molecular dynamics is a growing scientific field, with applications in materials sciences, biology and chemistry. Simulations at the atomic scale are now consuming huge computational resources and new algorithms to perform efficiently such simulations are proposed on a daily basis. We will present a few scientific challenges raised by such computations, and how mathematics can help to deal with them.

Tuesday 10:00 Highlight Talk 4

Microscopy – where modelling meets reality

Richard Beanland

High energy electrons have wavelengths of a few picometres and have a strong interaction with matter. This allows very small amounts of material to be examined using electron microscopy. Transmission electron microscopy (TEM) allows the interior of materials to be examined, and now provides atomic resolution data (e.g. Fig. 1) on a regular basis. Furthermore, in combination with electron diffraction, X-ray spectroscopy and electron energy-loss spectroscopy, elemental and chemical information can also be obtained at the nanometre or atomic level.

The macroscopic properties of materials are often dictated by processes that take place at microscopic length scales, which are often modelled using atomistic modelling techniques including DFT and molecular dynamics as well as phase field simulations and continuum models. Often, the validity of these models – and their ability to correctly predict material properties – can only be tested by comparison with atomic resolution data. Furthermore, the observed behaviour of materials can be unexpected, with structures that would be hard to imagine even with detailed knowledge of the materials.

This talk will give examples of recent work in Warwick microscopy that has linked with modelling as well as others that present interesting problems that could be tackled in the future.

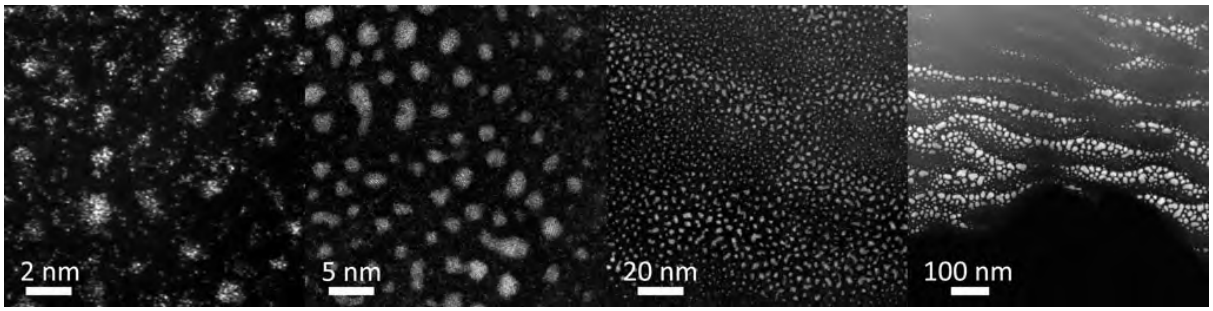

Figure 1. Scanning transmission electron microscope (STEM) images of Cu electrodeposited onto a boron-doped diamond substrate. Individual atoms and small clusters can be seen on the left. Although the deposition looks homogeneous at the scale of a few nanometres, on the scale of tens or hundreds of nm there are large variations in the amount of material deposited and the size of the Cu particles.

Tuesday 14:00 Highlight Talk 5

Molecular simulations you can trust and reproduce: The OpenKIM framework

Ryan S. Elliott, Ellad B. Tadmor

The quality of classical molecular and multiscale simulations hinges on the suitability of the employed interatomic model (IM) for a given application. Reproducibility of simulations depends on the ability of researchers to retrieve the original IM that was used. These two issues are addressed by the Open Knowledgebase of Interatomic Models project (https://openkim.org). OpenKIM curates IMs with full provenance control, issues them DOIs so that they can be cited in publications, and tests them exhaustively using "KIM Tests" that compute a host of material properties and "Verification Checks" on coding correctness. OpenKIM is integrated into major simulation packages (including ASE, DL_POLY, GULP and LAMMPS) allowing users to easily use OpenKIM IMs and query their predictions. Machine learning based tools for selecting an IM and assessing uncertainty are under development. OpenKIM functionality provides major benefits to researchers and promises to improve the reliability and reproducibility of molecular simulations of materials.

Guidelines for co-creation of PhD project outlines

The aim of this session is to work in mixed groups to come up with one or more short outlines that describe potential PhD projects, either for a 2020 start or in the longer term. Identify a spokesperson who will present the outcome of your group's discussion back to the whole group on Tuesday morning.

Projects will be considered for advertising for an October 2020 start. Those that attract match funding will be prioritised. (Overall, we are aiming for around 4 externally supported projects per cohort to attract 50% match funding of £50k – £12.5k per year over the 4 years of the PhD).

Some questions to consider for each project:

What are the research challenges and where do they go beyond current state-of-the-art?

Why is a HetSys PhD the right way to address these challenges?

What will be the main outcome of the PhD after 4 years?

How does the project align with the 3 HetSys training objectives?

1. spans discipline boundaries
2. incorporates uncertainty into modelling
3. promotes robust software engineering

How will the project benefit from the HetSys training programme?

Specify one or more research areas for the project. These could be one or more of the 8 HetSys research themes listed on the HetSys website:

1. Novel electronic devices
2. Catalysis
3. High performance alloys
4. Direct drive laser fusion
5. Future medicines
6. Smart nanofluidic interfaces
7. Composite materials
8. Underground systems

Are there potential partners – either existing or new?

- Industrial
- International
- Experimental

Who would be the academic supervisors/co-supervisors?
(At least two, from different departments/disciplines/research methodologies)

Who would be mentors/supporters at the project partner?

Is there a proof of principle/some initial data available?

How will knowledge be exchanged between partners during project and beyond?

What future collaborations/projects could this PhD project lead to?