HETSYS MATTERS

Engineering and Physical Sciences Research Council

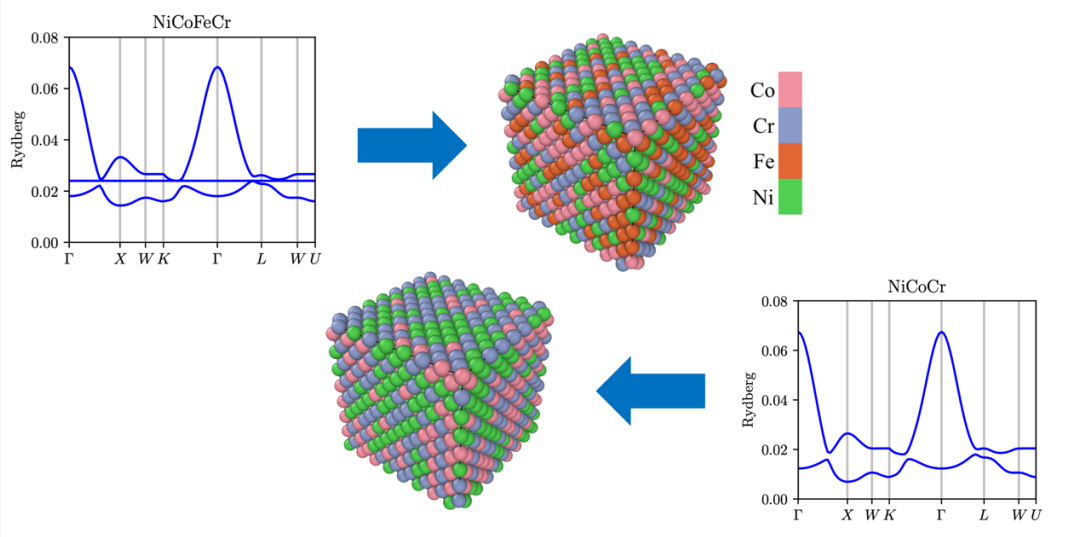
NEWS FROM THE EPSRC DOCTORAL TRAINING CENTRE IN THE MODELLING OF HETEROGENEOUS SYSTEMS (HETSYS)

HetSys research features in *Physical Review B*

Latest work by Christopher Woodgate and Julie Staunton is featured as an Editors' Suggestion in the latest edition of *Physical Review B*.

Using a combination of density functional theory (DFT) calculations, a linear response theory, and atomistic simulations, this paper studies the nature of short- and long-range order (S/LRO) in the prototypical high entropy alloy (HEA), NiCoFeMnCr, and its derivatives, collectively referred to as the Cantor-Wu alloys.

The calculations represent the first implementation of the linear response theory, based on a Landau-type expansion of the free energy of the system around a disordered, homogeneous reference state. The theory is able to predict second-order phase transitions directly, obtaining both the temperature at which the transition occurs as well as the leading pairwise correlations associated with which it is associated. In addition, pairwise parameters suitable for atomistic modelling at longer length scales are obtained and employed successfully to provide more intuitive insight into the nature of SRO in these materials.



INSIDE

The calculations are in good agreement with existing literature, both theoretical and experimental, but employ only a few hundred CPU hours, while existing literature often use significantly more resources to obtain the same results. The paper was selected as an 'Editors' Suggestion' for a recent edition of Physical Review B.

The paper serves as validation of the approach to modelling compositional order in multicomponent alloys, and the intention is now to move on to studying other multicomponent systems with magnetic applications.

Christopher D. Woodgate, Julie B. Staunton,
"Compositional phase stability in medium-entropy and high-entropy Cantor-Wu alloys from an ab initio all-electron Landau-type theory and atomistic modelling"
Phys. Rev. B, 105 115124 (2022).
DOI: https://doi.org/10.1103/PhysRevB.105.115124

HetSys People

CONGRATULATIONS TO...

Idil Ismail for her Iota Sigma Pi #BlackinChem Travel Award.

Established in 1902, **Iota Sigma Pi** aims to promote the advancement of women in science, especially Chemistry. For the second year running, Iota Sigma Pi has participated in **#BlackinChem** week by awarding a $500 travel award to a woman graduate student.

#BlackInChem was founded in 2020 inspired by a series of "BlackinX" events and works hard to connect Black chemists in the US and Europe, and has catalysed a conversation regarding the need for greater representation of Black chemists. Idil's poster: "***Automating the Prediction of Chemical Reactions using stochastic graph-based methods coupled with machine learning architecture***" was presented online as part of the #BlackinChemPosterComp 2021.

Kat Blow's work featured as an 'Editors Choice' in the Journal of Chemical Physics

The Journal of Chemical Physics (JCP) produces some of the most innovative and influential articles in chemical physics and physical chemistry each year. Kat Blow's latest paper ***"The seven deadly sins: When computing crystal nucleation rates, the devil is in the details"*** written with her supervisors Gabriele Sosso and David Quigley, has been selected for JCP Editors' Choice 2021, a special edition of the journal which features papers that present significant and definitive research in experimental and theoretical areas of the field.

Nucleation of materials is important in many industries, including pharmaceutical and oil. However, it is still poorly understood and computer simulations compute nucleation rates which differ from both experiment and other simulations by orders of magnitude. In their paper Kat, Gabriele and David put forward several factors which may play important roles in this discrepancy.

Katarina E Blow, David Quigley and Gabriele C Sosso
The seven deadly sins: When computing crystal nucleation rates, the devil is in the details.
J. Chem. Phys. **155**, 040901 (2021). [Editor's Pick]
DOI: https://doi.org/10.1063/5.0055248

First HetSys PG Diplomas awarded

The HetSys integrated training programme includes a taught element which leads to a Postgraduate Diploma.

We are delighted to announce that the first cohort of HetSys students have all successfully completed their Postgraduate Diplomas and all graduated in absentia in January 2022.

Due to Covid-19 restrictions, we were unable to celebrate in person, but look forward to coming together in the summer to toast the student's hard work and success.

The prize for best overall performance has been awarded to Andrew Angus.

Congratulations, Cohort 1!

HetSys Presents...

Some recent conference presentations by HetSys students:

Connor Allen (cohort 2) presented: "*Gaussian Approximation Potentials for Ti based alloys - Data generation for better phonon representation*" at the **AWE Materials and Analytical Student Conference 2022**

Andrew Angus (cohort 1) presented "*Machine-Learning Methods for Modelling Laser-Plasma Interactions in ICF*" at the **A141CF Meeting**

Jingbang Liu (cohort 1) presented "*Modelling of Confined Nanoscale Thin Films*" at the **British Applied Mathematics Colloquium**

Kat Blow (cohort 1) presented "*One Dimensional Crystal Nucleation Rates*" at the **RSC Faraday Conference**

Idil Ismail (cohort 1) presented "*Automating the Prediction of Chemical Reactions using stochastic graph-based methods coupled with machine learning architecture*" at the **American Chemical Society Spring Meeting**

HetSys Outreach

HetSys is passionate about sharing our research and our expertise. Whether we are supporting schools, or working with Industry we want to make sure we have an impact in the real world.

Most recently, our students have launched an online seminar series "**The Computational Toolkit**" which features PhD students from HetSys and associated CDTs giving short talks on key computational skills used in everyday research to create a so-called "computational toolkit" of resources and tutorials. The series is aimed at helping those just beginning in the field, and offers a practical introduction to computational science as a whole. It will cover a range of topics relevant to someone who's just taking an interest in computational science as a whole, or someone who might be looking for more information on a specific a programming tool,

The seminars are being streamed live via Youtube each Tuesday at 1600 GMT. For full details including links to join and a schedule please visit the Computational Toolkit website or contact hetsys@warwick.ac.uk for more information.

HetSys Outreach Activity is coordinated and by a committee of students and convened by Dr Mohad Mousavi-Nezhad. For more information, please visit the Outreach pages on the HetSys website.

INTERNATIONAL DAY OF WOMEN AND GIRLS IN SCIENCE

In February, we celebrated the International Day of Women and Girls in Science by hosting a campaign on our twitter account (@HetSysCDT) highlighting some of the fantastic women who work in our Centre.

UNESCO and UN-Women founded the International Day of Women and Girls in Science in 2015. Since then, each year on 11 February the critical role that women and girls play in science and technology is both recognised and celebrated internationally.

You can read the Women in the Physical Sciences case studies on our IDWGS 2022 website

MULTISCALE MUSINGS PODCAST

Multiscale Musings is a podcast series all about computational science multi-scale modelling of heterogeneous systems. It is produced and presented by PhD students from the Hetsys CDT and features interviews with promenent academics whose research relates to the key themes of HetSys

The Podcast has now concluded it's second season and plans are underway for a third. You can still listen to all 16 episodes via Spotify or Mixcloud. Visit the Multiscale Musings website for links and further information or follow on Twitter via @MultiscaleMuse

HetSys solves "real-world" problems at the 2022 Industry Study Event

From 4th to 6th April 2022, HetSys CDT students, together with staff and students from across the Faculty, took part in an Industry Study Group on campus at Warwick. Challenges were posed by **Dassault Systèmes BIOVIA**, **TWI Ltd** and **Bayer AG**, focussing on uncertainties in Molecular Dynamics Simulations, corrosion in "Slugcatchers" used in the oil and gas industry, and the absorption of Plant Protection Products (PPPs) in soils, respectively.

Students worked together intensively with input from the industry partners and staff to devise, model, code and compute solutions to the challenges, before presenting their results back to the group at the end of the event.

HetSys Director, **Julie Staunton** said:

> *The event really demonstrated the true interdisciplinary nature of HetSys. It was fantastic to sense the enthusiasm and to see our students pooling their expertise to solve these problems in innovative and exciting ways*

Felix Hanke from Dassault Systèmes BIOVIA commented that:

> *It was great to see so many different solution approaches to our challenge, and to learn from students and staff alike. I really hope that we can use this opportunity as a start for a longer term collaboration with HetSys.*

Tom Rocke, who is a first year PhD student within HetSys, worked on the challenge set by Dassault Systèmes BIOVIA and said:

> *The most valuable part of the Industry Study Event to me was being able to apply the techniques which we study in the HetSys training on a Real World problem. Applications of techniques used in lectures and workshops are often curated to give nice neat results as a demonstration tool, so it was stimulating to work on a problem where the path forward was less obvious.*

Study Groups like these have been hugely successful in solving problems and providing insight for various organisations. Previous events have pump-primed current co-funded HetSys PhD projects with AWE and Astra Zeneca.

We would like to offer our thanks to the **Knowledge Transfer Network** and the **EPSRC Impact Acceleration Account** for supporting this important event, and of course to our colleagues from Dassault Systèmes BIOVIA, TWI Ltd and Bayer AG for their time and input.

HPC REPROHACK @ WARWICK

With support from the EPSRC, HetSys partnered with the ReporoHack foundation to develop the first **High Performance Computing 10-day ReproHack event** in March.

The aim of the extended event was to reproduce the findings of computationally intensive published research from associated code and data on the Sulis Tier 2 HPC system and feedback their experiences to authors as well as the group of participants.

Aravinthen Rajkumar, a third year HetSys student participated in the event and said:

> *I found the Reprohack to be an excellent means of communicating the importance of reproducibility in computational science - participating in the event has left a genuine and lasting impact on the manner in which I write my own scientific code.*

SAVE THE DATE!

The Hetsys Summer Conference will be held on 19th and 20th July 2022 on the University of Warwick campus

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