# Theory of Condensed Matter Group Scientific Meeting

## University of Warwick, Thursday 16th June 2022

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| 10.30 | Arrival and Coffee |
| 11.00 | Camille Scalliet, Cambridge,<br>*30 milliseconds in the life of a supercooled liquid* |
| 11.50 | Mohammad Saeed Bahramy, Manchester,<br>*Magnetic Generation and control of topological quantum phases in cross-correlation electron systems* |
| 12.40 | Lunch |
| 13.40 | Andrew Green, UCL<br>*NISQ Simulation and Machine Learning with Tensor Networks* |
| 14.30 | Sam Edwards Prize Presentation & Talk |
| 14:45 | Posters (including student poster prize) with tea at 15.30 |
| 16.20 | Oindrila Deb, Bristol<br>*Hunting Majorana Bound States in Topological Systems* |
| 17.10 | Close |

The meeting will be held off the Warwick Science Concourse.
*The ordering of speakers is subject to revision.*

Organised by Marcin Mucha-Kruczynski (Bath), Elsen Tjhung (Open), and Nicholas d'Ambrumenil (Warwick)

**Registration** + further details: theory.warwick.ac.uk/events/iop2022

IOP Institute of Physics
Theory of Condensed Matter Group

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# Posters

1. Measuring the adiabatic Non-Hermitian Berry Phase in Feedback-Coupled Oscillators, Yaashnaa Singhal, **Enrico Martello**, Shraddha Agrawal, Tomoki Ozawa, Hannah Price and Bryce Gadway, Birmingham
2. Quantum Information is a Hydrodynamic Slow Mode, Ewan McCulloch, Birmingham
3. Weyl-like points at the surface of NbGeSb: when the orbital angular momentum winds, Chris Hooley (St Andrews),Sankhya Basu (CUNY), Daniel Arovas (UCSD], Sarang Gopalakrishnan (Penn State), and Vadim Oganesyan (CUNY)
4. Incommensurate time crystals in non-unitary quantum circuits and the link to complex-temperature statistical mechanics, Chris Hooley, St Andrews
5. Machine Learning Random Structure Searching for Li-Ni-S Cathode Discovery, Jordan Durrell, University of Birmingham
6. Short-Range Order in High-Entropy Alloys: First Principles Theory and Atomistic Modelling, Chris Woodgate and Julie Staunton, Warwick

   Short-Range order (SRO) can be either beneficial or detrimental to the properties of novel high- and medium-entropy alloys. An understanding of phase behaviour and underlying physical mechanisms driving ordering is therefore essential. We present results from an all-electron, first principles, Landau-type theory which enables us to obtain SRO directly, and also to obtain parameters suitable for atomistic modelling to understand incipient order in these materials. As a case study, we present results on the prototypical face-centred cubic high-entropy alloy, NiCoFeMnCr, and its derivatives, collectively referred to as the Cantor-Wu alloys. We are able to show that the dominant correlations in these systems are between Co and Cr, and that Fe and Mn dilute interactions and stabilise the disordered solid solution.

7. $Ti_3C_2S_2$MXeneforanode electrode inMg-ion Batteries, Ti3C2S2MXeneforanode electrode inMg-ion Batteries, Coventry University
8. Li-ion mobility in variously terminated Ti3C2 MXene, Konstantina A. Papadopoulou and Stavros-Richard G. Christopoulos, Coventry University
9. Bloch Oscillations Along a Synthetic Dimension of Atomic Trap States, Christopher Oliver, Aaron Smith, Thomas Easton, Grazia Salerno, Vera Guerrera, Nathan Goldman, Giovanni Barontini, Hannah M. Price, Birmingham
10. Machine learning the 2D percolation model, Djena Bayo, Warwick
11. Electron-phonon decoupling in two dimensions, George McArdle and Igor Lerner, Birmingham
12. Lifshitz transition-induced tuning of charge density waves in 2H-TaSe2, Yiwei Li (Shanghai), William Luckin (Bath), Juan Jiang (Shanghai & Hefei), Surani M. Gunasekera (Bath), Dharmalingam Prabhakaran (Oxford), Felix Flicker (Cardiff), Yulin Chen (Oxford, Shanghai) and Marcin Mucha-Kruczynski (Bath) Will Lukin (Bath)

13. DFT exploration of the family of 2D metal organic frameworks M(C4N2H4)Cl2, Andrea Iliceto, Birmingham
14. Excited State Machine Learning for Chromophores in Complex Environments, Carlo Maino, Natercia d. N. Rodrigues, Vasilios G. Stavros, and Nicholas D. M. Hine, Warwick
15. Quantum Information is a Hydrodynamic Slow Mode, Ewan McCulloch, Birmingham
16. Quantifying the breakdown of electronic friction theory during molecular scattering of NO from Au(111), Connor L. Box (Warwick), Yaolong Zhang (Hefei), Rongrong Yin (Hefei), Bin Jiang (Hefei), and Reinhard J. Maurer (Warwick)

    The Born-Oppenheimer approximation fails to capture the extent of multiquantum vibrational energy loss recorded during molecular scattering from metallic surfaces. Vibrational state-to-state scattering of NO on Au(111) has been one of the most studied examples in this regard, providing a testing ground for developing various nonadiabatic theories. The exact failings compared to experiment and their origin from theory are not established for any system, particularly since dynamic properties are affected by compounding simulation errors, of which the quality of nonadiabatic treatment is just one. We use a high-dimensional machine learning representation to perform a comprehensive quantitative analysis of the performance of molecular dynamics with electronic friction in describing nonadiabatic state-to-state scattering. We find that electronic friction theory accurately predicts vibrationally elastic and weakly inelastic scattering, but underestimates vibrational inelasticity that involves multi-quantum energy loss and overestimates molecular trapping at high vibrational excitation. Our analysis reveals potential remedies to these issues.

17. Coarse-grained measurements and entanglement transitions, Oliver Lunt & Curt von Keyserlingk, Birmingham
18. Towards 2D Topological Chiral Orbits with a Synthetic Dimension of Atomic Trap States, **David Reid**, Christopher Oliver, Aaron Smith, Thomas Easton, Grazia Salerno, Vera Guarrera, Nathan Goldman, Giovanni Barontini, and Hannah Price, Birmingham