

Condensed Matter Theory Journal Club/PHY663/PHY363

S. Winter, A. R. S. Kandada, W. C. Kerr, T. Thonhauser, and N. A. W. Holzwarth

Fall 2024 Schedule: Fridays at 11:00-12:00 AM in Olin 105

To sign up for a talk, please edit this googledoc directly to add or change schedule or contact natalie@wfu.edu

- August 30, 2024 – Short presentations by participants describing highlights of summer 2024
- September 6, 2024 – Continued Short presentations by participants describing highlights of summer 2024
- September 13, 2024 – Ramesh Dhakal – “Berry phase, Berry curvature and topology in solids”
- September 20, 2024 – Group discussion led by Natalie on several seminal papers related to a component of “Machine Learning” and efficient functional representations of multicomponent potential energy surfaces. Two papers for the discussion are by [Behler and Parrinello](#) and by [Bartok](#).
- September 27, 2024 -- **postponed due to unpredictable weather**
- October 4, 2024 – Cory Lynch – “Improving First Principles Predictive Capabilities through the Implementation of Neural Networks and Machine Learned Interatomic Potentials”
- October 11, 2024 – Owen Ganter - “DMET versus pDMET: A Comparison of the Two Methods” Reference: [Wu et al.](#)
- October 18, 2024 – Fall break
- October 25, 2024 -- Dr. Sean Anderson will talk about and demonstrate the many **new developments in the DEAC cluster**
- November 1, 2024 – Samuel Griffith – “Details of The Kosterlitz-Thouless Transition”
- November 8, 2024 -- Katie Koch – “Modulating exciton polaron

characteristics via organic cation substitution in Ruddlesden Popper metal halides”

- **November 15, 2024 -- Trevor Jenkins –”Characterizing Molecular Physisorption in Metal-Organic Frameworks Using Density Functional Theory.”**
- **November 22, 2024 –Wells Graham – “Selective Adsorption and Diffusion in MOF NU2100”**
- **November 29, 2024 -- Thanksgiving Holiday**
- **December 6, 2024 – Banasree Sarkar Mou –"Evidence for a single-layer van der Waals multiferroic".**