

Condensed Matter Theory Journal Club/PHY663/PHY363

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Fall 2023 Schedule: Fridays at 1:00-2:00 PM in Olin 105

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

- September 1, 2023 – Organizational meeting with lunch and possibly phonon report by Natalie and Cory regarding a comparison of density functional perturbation vs. finite differences methodologies with thanks to Saif Ullah for his help.
- September 8, 2023 – Discussion of paper by Jianhang Xu, Yosuke Kanai, & colleagues on “First-Principles Approach for Coupled Quantum Dynamics of Electrons and Protons in Heterogeneous Systems” – <https://doi.org/10.48550/arXiv.2307.15598>
- September 15, 2023 – Continued discussion of the work of our colloquium visitors for Dec. 7th, with the additional more general articles on the breakdown of the Born-Oppenheimer approximation <https://doi.org/10.1063/PT.3.5172>, and of the methodologies of arXiv paper – <https://doi.org/10.1063/5.0088427> and <https://doi.org/10.1063/5.0066753>.
- September 22, 2023 – Ajay Ram Srimath Kandada will lead a discussion on research in the “Quantum UFOs Lab” of his group and opportunities for collaboration.
- September 29, 2023 -- Dominique Itanze will lead a discussion on “Mechanistic insights of butanol formation from electroreduction of CO₂ on CuP₂ “
- October 6, 2023 – Trevor Jenkins will lead a discussion on a recent paper “The borderless world of chemical bonding across the van der Waals crust and the valence region” by Jorge Echeverria and Santiago Alvarez – <https://doi.org/10.1039/D3SC02238B>
- October 13, 2023 – Fall break
- October 20, 2023 -- Owen Ganter will lead a discussion of “Introduction to Density Matrix Embedding Theory”. A relevant references is given in <https://doi.org/10.1103/PhysRevLett.109.186404>
- October 27, 2023 -- Ramesh Dhakal will lead a discussion of "Achilles' heel of Kitaev-spin liquid phase".
- November 3, 2023 -- Tim Carlson will lead a discussion on "Investigating the Utility of Resonator Circuits as the Host for Quantum States Thought to be Present at Room Temperature." Tim recommends the following articles relevant to his discussion -- <https://www.nature.com/articles/nature13171> and <https://ieeexplore.ieee.org/document/9789946>

- November 10, 2023 -- Cory Lynch will present "Machine Learning Based Molecular Dynamics" which he has recently started working on, based on the literature paper <https://doi.org/10.1038/s41467-023-36329-y>.
- November 17, 2023 -- Wells Graham will present "Water Sorption Modulation by Tuning Pore Chemistry and a continuation of our discussion of Machine Learned Interatomic Potentials" This will be an interesting combination of his current research projects and continuing some of the machine learning ideas from last week. Reference: <https://doi.org/10.1021/acs.jpcllett.0c01061>
- November 24, 2023 -- Thanksgiving Holiday
- December 1, 2023 -- Banasree Sarkar Mou will present "Optical matrix elements for nonlinear spectroscopy". A reference for this topic is "Principles of Nonlinear Optics and Spectroscopy" by Shaul Mukamel (1999) <https://mukamel.ps.uci.edu/index.html>
- December 8, 2023 -- Meeting with Deac Cluster Administrators