

# Condensed Matter Theory Journal Club/PHY663/PHY363

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## Fall 2022 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](mailto:natalie@wfu.edu)

- August 29, 2022 – Organizational meeting with lunch
- September 9, 2022 – Natalie Holzwarth will coordinate a discussion about useful resources for condensed matter research available on the internet – such as The Materials Project – <https://materialsproject.org/>, The Bilbao Crystallography Server <https://www.cryst.ehu.es/>, ICSD (Inorganic Crystal Structure Database) <https://icsd.fiz-karlsruhe.de/>, and many others. Going forward, please use/comment on/add to the shared Google Doc Website List – <https://docs.google.com/document/d/1pune26mrKOhCBJXAIB2BjWa5Lrmw5gcBCPtj7ccEbwo/edit?usp=sharing>
- September 16, 2022 – Stephen Winter will make a tutorial presentation in order to introduce quantum magnetism and spin liquids.
- September 23, 2022 -- Owen Ganter and Chao Shang - "Investigation of the Magnetic and Electronic Structure of Iridium Tetrafluoride"
- September 30, 2022 -- Dominique Itanze – Presentation of slides pertaining to ECS poster on "*Understanding the Mechanism of Butanol Formation from CO<sub>2</sub> Reduction on Phosphorus Rich Copper Catalyst, CuP<sub>2</sub>, by Computer Simulations Based on Joint Density Functional Theory*" and background literature discussion on "The electrochemical interface in first-principles calculations" by K Schwarz and R Sundararaman DOI: 10.1016/j.surfrep.2020.100492
- October 7, 2022 – Cory Lynch – Practice talk for ECS meeting in Atlanta GA on Oct. 9, 2022 – "Simulations and Analyses of Li<sub>4</sub> and Li<sub>6</sub> Boracites and Thioboracites As Promising Li Ion Conducting Electrolytes"
- October 14, 2022 – Fall break
- October 21, 2022 -- Haardik Pandey – "An overview of Conducting Metal Organic Frameworks based on the publication from the website [Electrically Conductive Metal–Organic Frameworks | Chemical Reviews \(acs.org\)](https://pubs.acs.org/doi/10.1021/acs.chemrev.9b00766). <https://pubs.acs.org/doi/10.1021/acs.chemrev.9b00766>
- October 28, 2022 -- Trevor Jenkins – "An overview of the new vdW-DF2-ahbr hybrid functional" as presented in the paper "Accurate Nonempirical Range-Separated Hybrid van der Waals Density Functional for Complex Molecular Problems, Solids, and

Surfaces" DOI: 10.1103/PhysRevX.12.041003

- November 4, 2022 -- Banasree Sarkar Mou – "Hopping integral and different methods of approaching it"
- November 11, 2022 -- Timothy Carlson – "Magnetic Force Microscopy of Topological Insulators- a Search for Persistent Current"
- November 18, 2022 -- Wells Graham – "Examining the Ethane Selective Potential of MOFs for Ethylene Purification" and Ramesh Dhakal – "Ab initio study of stable 3d, 4d, and 5d transition-metal-based quaternary Heusler compounds"
- November 25, 2022 -- Thanksgiving Holiday
- December 2, 2022 -- Saif Ullah – "Water and CO<sub>2</sub> coadsorption in TIFSIX-3-Ni: A duel or a duet?"