PHY556 Project Assignments: Journal Club

This document outlines the final project assignments for PHY556 in the form of a journal club. Each student will present and lead a discussion on a selected research paper. Papers are grouped by topic and aligned with different student interests (theoretical vs applied).

1. Quantum Embedding Methods

- **Density Matrix Embedding Theory (DMET):**
  Knizia & Chan, "Density matrix embedding: A simple alternative to dynamical mean-field theory," PRL **109**, 186404 (2012).

- **Self-Energy Embedding Theory (SEET):**
  Zgid & Gull, "Tractable self-consistent auxiliary-field method for correlated electrons in realistic materials," NJP **19**, 023010 (2017).

- **DMET in Quantum Chemistry:**
  Wouters et al., "Practical guide to density matrix embedding theory in quantum chemistry," J. Chem. Theory Comput. **12**, 2706 (2016).

2. Quantum Monte Carlo Applications

- **Hydrogen Phase Diagram:**
  McMahon et al., "The properties of hydrogen and helium under extreme conditions," Rev. Mod. Phys. **84**, 1607 (2012).

- **QMC Benchmarking DFT:**
  Morales et al., "Nuclear Quantum Effects and Nonlocal Exchange-Correlation Functionals Applied to Liquid Hydrogen at High Pressure," PNAS **107**, 12799 (2010).

- **QMC for Solids:**
  Hennig et al., "Quantum Monte Carlo calculations of semiconductors using twist-averaged boundary conditions," PRB **82**, 014101 (2010).

3. DMFT Applications to Correlated Solids

- **Cluster DMFT in V_2O_3:**
  Park, Haule & Kotliar, "Cluster DMFT study of the Mott transition in V_2O_3," PRL **101**, 186403 (2008).

- **Nickelates from First Principles:**
  Chen et al., "Modelling the rare-earth nickelates from first principles," NPJ Quantum Materials **5**, 44 (2020).

- **FeO and Metal-Insulator Transition:**
  Leonov et al., "Metal-insulator transition and magnetism in correlated band insulator FeO from dynamical mean-field theory," PRL **101**, 096405 (2008).

4. GW and Beyond

- **Self-Consistent GW in Solids:**
  Shishkin & Kresse, "Self-consistent GW calculations for semiconductors and insulators," PRB **75**, 235102 (2007).

- **Benchmark of GW Methods:**
  Caruso et al., "Benchmark of GW methods for solids," PRB **90**, 085141 (2014).

- **GW for Molecules:**
  Blase, Attaccalite & Olevano, "First-principles GW calculations for molecules," PRB **83**, 115103 (2011).

5. Benchmarking Project: Band Gap of Silicon

Objective Compare the quasiparticle gap of crystalline silicon using:

- DFT (e.g., LDA or GGA)
- GW (G_0W_0, GW_0, scGW)
- Quantum Monte Carlo (DMC or AFQMC)
- Experimental data

Assigned Papers

- *Shishkin & Kresse*, PRB **75**, 235102 (2007) – GW treatment.
- *Hennig et al.*, PRB **82**, 014101 (2010) – QMC approach.
- *Caruso et al.*, PRB **90**, 085141 (2014) – Comparison across GW variants.

Tasks

1. Extract and tabulate calculated band gaps from each method.
2. Compare with experimental optical/photoemission values.
3. Discuss physical reasons for discrepancies: e.g., self-interaction error, missing screening, sign problem.
4. Reflect on cost vs accuracy trade-offs for each method.