

# CONDENSED MATTER SCIENCES SEMINAR

## Professor Eugene De Prince

Florida State University

### Host

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### Title

Lower Bounds in Quantum Chemistry

Friday, May 8<sup>th</sup>, 2026

1<sup>st</sup> Floor – B101

15:00-16:00

### Abstract

Any electronic Hamiltonian can be decomposed into a sum of squares (SOS) of products of fermionic creation and annihilation operators plus a constant shift. The constant shift is a lower-bound to the ground-state energy of the Hamiltonian, and a tighter lower-bound can be obtained as the pool of fermionic operators becomes more complete. The SOS decomposition problem is a complement to a more well-known approach in quantum chemistry based on the variational optimization of the two-electron reduced density matrix (2RDM). In this approach, the 2RDM is optimized subject to a set of ensemble N-representability conditions, and, as the set of conditions becomes more complete, the trace of the 2RDM against the Hamiltonian approaches the full configuration interaction energy from below. In this talk, I will discuss the similarities and differences between the SOS and variational 2RDM approaches.