Speaker: Srinivasa Prasannaa V, Associate Professor, TCG Crest, Kolkata, India

Time and venue: August 20, 2026; 4:00 PM; Physics Seminar Hall HSB-209, Dept. of Physics

Title: Quantum computing and its applications to atomic and molecular physics

Abstract: Quantum computing offers new approaches to solving challenging quantum many-body problems in atomic and molecular physics, where the exponential growth of the Hilbert space can limit conventional computational methods. In this seminar, I will discuss our recent work on quantum algorithms and their applications to electronic-structure calculations, spanning both NISQ and fault-tolerant quantum computing. I will begin with variational and sampling-based approaches, including the variational quantum eigensolver (VQE) [1,2], quantum annealing [3], and quantum-selected configuration interaction (QSCI) [4]. I will then focus on our work with quantum linear solvers, particularly the Harrow–Hassidim–Lloyd (HHL) algorithm and its applications to atomic and molecular systems, including adaptations such as AdaptHHL and PsiHHL. I will discuss the structure of the resulting linear systems and examine the prospects for quantum advantage using quantum linear solvers [5]. Finally, I will outline directions toward practical quantum simulations of strongly correlated atomic and molecular systems.

References:

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[2] A. Kalam, P. Deb, A. Sakurai, B. K. Sahoo, V. S. Prasannaa, and B. P. Das, Phys. Rev. Research 8, 023272 (2026).
[3] Aashna Anil Zade, K. Sugisaki, M. Werner, A. Palacios, A. Garcia-Saez, A. Riera, and V. S. Prasannaa, EPJPlus 140, 930 (2025).
[4] S. Sahoo, A. Kalam, K. Sugisaki, V. S. Prasannaa, and B. P. Das, arXiv2607.27777 (2026).
[5] D. Shetty, S. Dutta, P. Chawla, A. Jayashankar, Jordi Riu, Jan Nogue, K. Sugisaki, and V. S. Prasannaa, Phys. Rev. A 113, 052402 (2026).