Contribution ID : **1** Type : **Oral Presentation**

Advancing the Scope of Natural Orbital Functional Theory

Natural Orbital Functional Theory [1,2] has emerged as a transformative framework for studying strongly correlated electronic systems, achieving an exceptional balance between accuracy and computational efficiency. Recent advancements have significantly broadened its applicability, driving breakthroughs in the analysis of large-scale systems, direct-dynamics simulations of chemical reactions, excited states, and quantum computing integration via the one-particle reduced density matrix (RDM).

This presentation will highlight an innovative optimization strategy that accelerates NOF calculations for large systems, enabling the study of unprecedentedly complex phenomena, such as the dissociation of a 1000-electron hydrogen cluster [3]. The discussion will also delve into insights from direct-dynamics simulations [4], supported by GNOF [5] calculations of the electronic structure, to analyze the making and breaking of chemical bonds in reactive processes. These simulations, combined with natural orbitals, elucidate the dynamical evolution of chemical bonds, as demonstrated in the F^- + CH3CH2Cl reaction [6].

Additionally, I will explore the use of NOFs in modeling excited states through the coupling of reconstructed two-particle RDM with the extended random-phase approximation, showcasing their accuracy across various systems when compared to configuration interaction method [7]. The integration of NOFs into quantum computing, particularly within the Variational Quantum Eigensolver (VQE) framework, will also be addressed, emphasizing how leveraging the one-particle RDM allows for energy calculations with up to 90% reductions in quantum resource requirements [8].

These advancements collectively position natural orbital functional theory as a cornerstone methodology for tackling challenges in electronic structure calculations, offering transformative capabilities across classical and quantum computational domains.

[1] M. Piris, “Advances in approximate Natural Orbital Functionals: From historical perspectives to contemporary developments”; Adv. Quantum Chem., 2024, 90, 15.

[2] M. Piris, “Exploring the Potential of Natural Orbital Functionals”; Chem. Sci., 2024, 15, 17284.

[3] J. F. H. Lew-Yee, J. M. del Campo, M. Piris. Phys. Rev. Lett., 2025; arXiv:2502.01786.

[4] A. Rivero-Santamaría, M. Piris. J. Chem. Phys., 2024, 160, 071102; arXiv:2311.04802.

[5] M. Piris. Phys. Rev. Lett., 2021, 127, 233001; arXiv:2112.02119.

[6] M. Piris, X. Lopez, J. M. Ugalde, J. Phys. Chem. Lett., 2024, 15, 12138.

[7] J. F. H. Lew-Yee, I. A. Bonfil-Rivera, M. Piris, J. M. del Campo. J. Chem. Theory Comput., 2024, 20, 2140; arXiv:2311.05504.

[8] J. F. H. Lew-Yee, M. Piris, J. Chem. Theory Comput., 2025, 21, 2402.

Primary author(s) : Prof. PIRIS, Mario

Presenter(s) : Prof. PIRIS, Mario