The Electron Nuclear Dynamics Method in the Age of Ion Cancer Therapy, Machine Learning, and Quantum Computing

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Electron nuclear dynamics (END) is a time-dependent, variational, on-the-fly, and non-adiabatic method to simulate various types of chemical reactions and scattering processes[1]. The simplest-level END (SLEND) featured herein describes the nuclei in terms of classical mechanics and the electrons with a single-determinantal wavefunction in the Thouless representation[1]. Over the years, the Morales group has substantially extended END, both in its theoretical and computational aspects[1, 2]; thus, a methodology initially designed to treat small molecular systems has evolved into a powerful tool that can treat biomolecules [1, 2]. More recently, the Morales group has succeeded in placing END on the front line of contemporary research, in such diverse areas as biomedicine, coherent states theory, machine learning, and quantum computing[1, 2]. In this talk, I will review our latest END developments in those areas that include: **(1)** SLEND simulations of various reactions occurring in ion cancer therapy (e.g., water radiolysis and ion-induced DNA damage)[2], **(2)** the development of novel types of rotational coherent states to reconstruct quantum rotational properties from classical dynamics[3, 4], **(3)** the development of analytical formulae to calculate electron-transfer probabilities via the Thouless coherent states[5], **(5)** the promotion of time-dependent symmetry breaking to improve SLEND simulations[6], **(6)** the development of machine learning algorithms for SLEND simulations, and **(7)** the formulation of END in the framework of quantum computing.

References

1. C. Stopera, T. V. Grimes, P. M. McLaurin, A. Privett and J. A. Morales, *Adv. Quantum Chem.*, 2013, **Vol. 66, Chapter 3**, 113-149.
2. E. Teixeira, K. Uppulury, A. Privett, C. Stopera, P. M. McLaurin and J. A. Morales, *Cancers*, 2018, **10**, 136.
3. C. Stopera and J. A. Morales, *J. Chem. Phys.*, 2020, **152**, 134112.
4. C. Stopera and J. A. Morales, *J. Chem. Phys.*, 2022, **156**, 224114.
5. E. D. Silva, P. M. McLaurin and J. A. Morales, *J. Chem. Phys.*, 2021, **155**, 124112.
6. P. M. McLaurin, R. Merritt, J. C. Dominguez, E. S. Teixeira and J. A. Morales, *Physical Chemistry Chemical Physics*, 2019, **21**, 5006.