New Frontiers in Multireference Molecular Simulations

Toru Shiozaki

Department of Chemistry

Northwestern University

Email: shiozaki@northwestern.edu

Abstract:
In this talk, I will describe a number of directions that our research group has pursued in the past few years. The first part summarizes the development of tensor-network ansatze based on the chemical structure, which we call active space decomposition. Second, I will talk about the development of CASPT2 nuclear gradients, which has enabled predictive on-the-fly photodynamics simulations. Finally I will present the development of the BAGEL program package and its software infrastructure.