

ID: 1.7.1b

Title: Ab initio simulations in quantum many-body systems by auxiliary fields

Name: Zhang, Shiwei

Affiliation: College of William and Mary, Williamsburg, VA, USA

Recent progress has made auxiliary-field quantum Monte Carlo (AFQMC) a promising general approach for ab initio simulations of ground-state properties of many-body systems. This was made possible by understanding and circumventing the sign problem in second-quantized orbital space, and by formulating effective importance sampling algorithms with auxiliary fields. I will discuss applications in three areas: in quantum chemistry where accurate energetics in molecular systems are systematically achieved; in materials physics when traditional density-functional total energy approaches are not effective; and in cold atoms and optical lattices where AFQMC is used to predict new phases.