

Materials Science and Technology Division
and
Computer Science and Mathematics Division

“State of quantum Monte Carlo”

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11:00 a.m.
5100, 128/JICS Auditorium

Abstract

With advances in algorithms and growing computing powers, quantum Monte Carlo (QMC) methods have become a leading contender for high accuracy calculations for the electronic structure of realistic systems. In this talk, I present recent developments in QMC theories and numerical algorithms which have allowed us to reach the necessary accuracies and system sizes with unprecedented time-to-solution. Also presented are the applications that highlight the strengths and limitations of QMC methods at present. Finally, I examine readiness of QMC in the era of materials design by quantum simulations.

Host: Fernando Reboredo (MSTD) and Bobby Sumpter (CSMD)