Engineering *ansatze* and cost functions for quantum simulations of molecular systems

Daniel Claudino

Computational Sciences and Engineering Division
Oak Ridge National Laboratory, Oak Ridge, TN

Satisfactory treatment of molecular states has proven to be a perennial challenge. Despite decades of success, there still remains a large divide between straightforward coupled cluster theory and strong correlated systems. These systems are postulated as the prime example to showcase computational advantage from quantum computers, but many are the reasons why it has yet to materialize. In this talk I will discuss how to draw inspiration from coupled cluster theory, particularly its unitary formalism, in the design of sensible *ansatze* that are easier for quantum computers to cope with and approximations to further alleviate such a burden. Concomitantly, I will also consider how this issue can be attacked by turning to alternative quantum observables and the underlying cost functions.