Chemical Engineering

Spring 2022 Seminar Series

http://cheme.mit.edu/seminar-series/

Challenging Problems in Quantum Chemistry: How to Diagnose Them and How to Tackle Them

Dr. Joonho Lee

Postdoctoral Researcher
Department of Chemistry
Columbia University

Thursday, February 3, 2022
4:15pm, 66-110
or via Livestream (link to be sent day of seminar)

ABSTRACT: Quantum chemistry has become an indispensable tool in revealing the microscopic details of molecules and materials such as barrier heights, interaction energies, and correlation functions. The nature of electronic correlation is sometimes controversial, obscuring the optimal choice of quantum chemistry methods with minimal computational effort and the desired accuracy. First, I will discuss a computational framework that addresses this question using regularized perturbation theory. Second, I will also discuss several challenging problems beyond the scope of such perturbation theory. I will argue that these problems can be tackled by methods based on auxiliary-field quantum Monte Carlo. Lastly, I will present my latest development of a new quantum-classical hybrid algorithm in this context, which represents the largest quantum computation of chemical systems on a quantum computer to date.