New frontiers of coupled-cluster theory: solid-state applications, anharmonic vibrational analog, finite-temperature extension, explicit correlation, automated implementation, and general-order algorithm

So Hirata

University of Illinois at Urbana-Champaign, Department of Chemistry, Urbana, IL 61801

We survey more recent extensions we made to coupled-cluster (CC) theory, some of which being motivated by its unique strengths such as size consistency, ability to treat metals, and forming a systematic sequence of increasing accuracy. They are (1) applications to one-dimensional solids with various measures to combat its immense computational cost, (2) the development of anharmonic vibrational CC, equation-of-motion CC (EOM-CC), and similarity-transformed EOM-CC (STEOM-CC) theories, (3) a finite-temperature extension and its applications to Peierls transition and metallic electronic structures, (4) explicitly correlated CC and combined CC and perturbation methods, enabling a near-exact solution of the Schrödinger equation, (5) automated formula derivation and parallel code synthesis for high-rank CC and EOM-CC methods, and (6) determinant-based, general-order CC and EOM-CC methods.