INTERMEDIATE HAMILTONIAN RELATIVISTIC MULTIREFERENCE COUPLED CLUSTER METHODS: THEORY AND APPLICATIONS

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Newly developed relativistic multireference Coupled Cluster (CC) schemes based on Intermediate Hamiltonian formulation are presented. This formulation widely extends possibilities of the traditional Fock-space and Hilbert-Space CC approaches.

High-precision calculations of some heavy and super-heavy atomic and molecular systems are presented. A detailed study of the influence of nonadditive effects of relativity and electron correlation on atomic and molecular properties is provided.