~90 Years of Relativistic Molecular Quantum Mechanics

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In this perspective talk on relativistic molecular quantum mechanics, I shall highlight the "history" of relativistic methods for the electronic structure of atoms, molecules and solids. Briefly, the foundation of relativistic quantum mechanics was established by Dirac in 1928, by combining quantum mechanics with the special theory of relativity. Yet, relativistic effect (i.e., any difference between the Dirac and Schrödinger equations) was widely recognized in chemistry and molecular physics only in the beginning of 1970's. Several approximate two-component (A2C) relativistic methods were developed between the mid of 1980's and the mid of 1990's, while exact two-component (X2C) relativistic methods were formulated between 2005 and 2009. An effective quantum electrodynamics (eQED) approach was also proposed a few years ago for QED effects in many-electron atoms and molecules. All in all, a complete and continuous "Hamiltonian Ladder" has been established, from which one can pick up the right Hamiltonian for the target physics and accuracy [Phys. Rep. 537, 59 (2014); Natl. Sci. Rev. 3, 204 (2016); Handbook of Relativistic Quantum Chemistry (Springer, 2017)]. Yet, the combination of relativistic Hamiltonians with many-body theories for the whole periodic table remains to be explored.