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Editorial

Special issue of Chemical Physics on recent advances and applications of relativistic quantum chemistry

As any difference between the Dirac equation describing our real world in which light travels at a finite speed and the Schrödinger equation describing an artificial world in which light travels infinitely fast, relativistic effects grow quadratically with respect to the binding nuclear strength parameter $Z\alpha$ and can hence strongly influence the chemical and physical properties of heavy elements or their compounds. Relativistic effects, in particular, spin–orbit couplings, may become sizable for electronically excited states even of light atoms. Relativistic quantum chemistry has thereby been one of the most active subfields of atomic and molecular physics ever since the early days of 1970s and eventually experienced a boom in the last 5 years or so. This is symbolized by the advent of exact two-component relativistic Hamiltonians, by the novel reformulations of relativistic theories for magnetic properties, by the efficient implementations of state-of-the-art correlation methods, by the accurate estimates of quantum electrodynamic and parity violating effects, and by the new examples demonstrating the importance of relativistic effects in our daily life. Yet, notwithstanding these successful stories, there still exist some fundamental questions on, e.g., how to define a proper relativistic many-electron Hamiltonian, how to formulate relativistic explicitly correlated methods to accelerate basis set expansions of the no-pair wave-function, how to go beyond the no-pair approximation so as to account for negative energy state contributions to correlation, and so on. All these topics were highlighted on the "9th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics" (REHE-2010) held in Beijing between September 25 and 29, 2010, during which the idea of this special issue was materialized. Based on the talks and posters presented in the conference, the papers are collected, to cover both the fundamentals of relativistic quantum chemistry and accurate results for the electronic structure, electric and magnetic properties of atoms, molecules and extended systems.

We thank all the authors for their contributions, Prof. Wolfgang Domcke for his support of this special issue, and the numerous referees for their efforts. We do hope that this collection will encourage the readers to think more commonly of relativity—It exists everywhere in your life.

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