Advances in Quantum Chemistry

Quantum Systems in Physics, Chemistry and Biology—Theory, Interpretation and Results

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Samantha Jenkins, Steven R. Kirk, Jean Maruani, and Erkki J. Brändas

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ADVANCES IN QUANTUM CHEMISTRY

Quantum Systems in Physics, Chemistry and Biology - Theory, Interpretation, and Results

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In this work an advanced relativistic quantum approach to computing the important radiative and collisional characteristics of multicharged ions in the Debye plasmas is presented. The approach is based on the relativistic energy formalism (the Gell-Mann and Low formalism) and relativistic many-body perturbation theory (PT) with the Dirac–Debye shielding model Hamiltonian for electron–nuclear and electron–electron systems. The optimized one-electron representation in the PT zeroth approximation is constructed by means of the correct treating the gauge-dependent multielectron contribution of the lowest PT corrections to the radiation widths of atomic levels. The computational results for the oscillator strengths and energy shifts due to the plasmas environment effect, the effective collision strengths for the Be- and Ne-like ions of Fe, Zn, and Kr embedded to different types of plasmas environment (with temperature 0.02–2 keV and electron density 10^{16}–10^{24} cm^{-3}) are presented and analyzed.. V. Buyadzhi, Vasily & A. Kuznetsova, Anna & A. Buyadzhi, Anna & V. Ternovsky, Eugeny & B. Tkach, Tatyana. (2018). Advanced Quantum Approach in Radiative and Collisional Spectroscopy of Multicharged Ions in Plasmas. 10.1016/bs.aiq.2018.06.002. In this work an advanced relativistic quantum approach to computing the important radiative and collisional characteristics of multicharged ions in the Debye plasmas is presented. The approach is based on the relativistic energy formalism (the Gell-Mann and Low formalism) and relativistic many-body perturbation theory (PT) with the Dirac–Debye shielding model Hamiltonian for electron–nuclear and electron–electron systems. The optimized one-electron representation in the PT zeroth approximation is constructed by means of the correct treating the gauge-dependent multielectron contribution of the lowest PT corrections to the radiation widths of atomic levels. The computational results for the oscillator strengths and energy shifts due to the plasmas environment effect, the effective collision strengths for the Be- and Ne-like ions of Fe, Zn, and Kr embedded to different types of plasmas environment (with temperature 0.02–2 keV and electron density 10^{16}–10^{24} cm^{-3}) are presented and analyzed.