Electron Correlation and Relativistic Contributions to Atomic and Molecular Electric Properties

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We will present and analyze results of all electron 'molecular' calculations of nuclear quadrupole moments of alkali metals and some other nuclei [1]. Electron correlation effects were accounted for at different levels of the approximation up to the CCSD(T) one. Relativistic effects were treated within the scalar Douglass-Kroll-Hess scheme. These results will be confronted with other available experimental and theoretical data. Special attention will be paid to the so-called picture change effect on expectation values of one-electron operators in the scalar relativistic approximation. This effect is expected to be particularly large for operators which assume large values in the vicinity of heavy nuclei.

We also will demonstrate how calculations of electric properties may help in the understanding of the differences between chemical bonds [2]. The series of molecules, like BMe, AlMe and FMe (Me = Cu, Ag, and Au) will be shown as an example. The analysis of molecular dipole moments and dipole polarizabilities serves as an alternative tool to the analysis of correlation and relativistic effects in chemical bonds along with the more traditional view through the relativistic effects on ionization potentials and electron affinities.

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