**Title: Quantum-mechanical non-Born-Oppenheimer calculations of small atoms and molecules.**

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**Abstract**

In this presentation I will describe the work carried out in my group concerning the development of quantum-mechanical methods for calculating bound states of small atoms and molecules without assuming the Born-Oppenheimer approximation. In the non-BO approach all particles forming the system (nuclei and electrons) are treated on equal footing. The energies of the states, which in the case of atoms include electronic ground and excited states and in the case of molecules include a combination of electronic and rovibrational states, are obtained in variational calculations using various types of all-particles explicitly correlated Gaussian (ECG) functions as basis functions. The wave function and the energy of each state is obtained in a separate calculation where its energy is minimized in terms of the non-linear parameters of the Gaussians. In the minimization, the analytically evaluated energy gradient determined with respect to the parameters is employed. This presentation is particularly focused on our works concerning the selection of ECG basis sets that enable non-BO calculations of atomic and molecular bound states with high accuracy.