Including Nuclear Quantum Effects in Computational Chemistry Calculations with Multicomponent Methods

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Nuclear quantum effects (NQEs) can be important in a variety of chemical phenomena including energy transfer, hydrogen bonding, and zero-point energy. Most computational chemistry calculations invoke the Born-Oppenheimer approximation, which separates the electronic and nuclear motion of the system. The Born-Oppenheimer is well justified for many chemical systems and is responsible for fundamental chemical concepts such as molecular orbitals and a potential energy surface, but it can lead to difficulty when including NQEs in computational chemistry calculations. In this talk, we will introduce a class of methods called multicomponent methods that can treat more than one type of particle quantum mechanically. Therefore, for molecular systems, the Born-Oppenheimer approximation is not invoked for (select) nuclei of the system, which simplifies the inclusion of NQEs. This leads to a concept of nuclear orbitals analogous to the familiar electronic molecular orbitals. We will show how multicomponent methods can be used to calculate accurate vibrationally averaged geometric properties and other chemical properties such as proton affinities. Recent improvements to multicomponent methodology including multicomponent selected CI and multicomponent CCSD(T) will be briefly discussed.