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Challenges in calculating molecular systems with Coulomb interactions NIKITA KIRNOSOV, KEEPER SHARKEY, LUDWIK ADAMOWICZ, Univ of Arizona — The highly accurate quantum mechanical calculations are not only crucial for high-resolution experimental data verification, but may also serve as a guide in the field of exotic systems exploration. Including all non-relativistic effects in a single-step variational approach and rigorously separating out the center of mass motion allows us to build a reliable model for calculating bound states of molecular systems with Coulomb interactions. In these calculations the wave function of the system is expanded in terms of explicitly correlated Gaussian (ECG) basis functions. Examples of calculations of energies and other properties of some molecular systems will be presented.

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