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**Complex explicitly correlated Gaussians for non-Born–Oppenheimer calculations of small molecules**[1]

SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — Non-Born–Oppenheimer calculations of molecular systems, where all particles are properly treated on an equal footing, represents a big challenge for the theory. Due to the huge difference in the masses of the electrons and nuclei the latter move more slowly and their correlation functions have distinct localization around the equilibrium internuclear separations. This feature is hard to implement in explicitly correlated variational approaches with Gaussian type basis functions while maintaining an analytic integrability of all necessary matrix elements. In this work we demonstrate that the difficulties can be overcome by using complex Gaussians. In our benchmark calculations on $HD^+$ molecular ion we have achieved excellent performance of this simple complex basis set that is on par or better than what was seen in previous Non-BO calculations of small diatomic molecules.

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