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Challenges and advances in calculations of highly non-adiabatic systems employing the explicitly correlated Gaussian functions NIKITA KIRNOSOV, The University of Arizona — Accurate calculations of the highly non-adiabatic systems have been drawing attention for several decades. While most accurate modern methods allow outstanding accuracy, they are limited to only three or four particles. In the current work we have developed a highly accurate method which is not limited by the number of particles in the system but is only limited by the computer resource available. Examples of calculations of exotic systems with[1] and without[2] rotational excitation and of conventional electronic molecules[3,4] are presented and the future development of the method is discussed.

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[3]K. L. Sharkey, N. Kirnosov and L. Adamowicz, J. Chem. Phys. **139**, 164119 (2013).
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