

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Perspectives and Current the Development of Non-Born-Oppenheimer Atomic and Molecular Quantum Mechanical Variational Calculations using Explicitly Correlated Gaussian Basis Functions¹

KEEPER L. SHARKEY, Univ of Arizona, ADAMOWICZ TEAM — The development of highly accurate theoretical quantum mechanics models for atomic and molecular calculations is crucial for the verification of the results of high-resolution experimental spectroscopy. High accuracy in the calculations can be achieved by not assuming the Born-Oppenheimer approximation (non-BO) and by using the variational principle. The non-relativistic Hamiltonian describing the internal state of the considered system used in the approach is obtained by separating out the center-of-mass motion from the laboratory frame Hamiltonian. The wave functions used in the calculations are expanded in terms of explicitly correlated Gaussian (ECG) functions. The optimization of the Gaussian non-linear parameters is aided by the analytical energy gradient determined with respect to these parameters. Examples of some very accurate calculations of small atoms and diatomic molecules will be presented. The presentation will also include a discussion of the extension of the approach to perform non-BO calculations of bound states of small triatomic molecules (e.g. H_3^+).

¹Acknowledgements go to Ludwik Adamowicz for guidance and NSF for funding (DGE1-1143953).

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Date submitted: 14 Nov 2013

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