Abstract Submitted
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DFT Calculation of the Renner Coefficient for the Renner-Teller Splitting in the NCO Radical: Assessing and Characterizing the accuracy of several common functional families and basis sets.[1] D. O. KASHINSKI[2], T. J. RADZIEWICZ, US Military Academy, E. F. C. BYRD, Army Research Laboratory — Assessment of "out of box" DFT methods through analysis of the Renner-Teller Effect on the NCO radical is underway. This student-centered project allows us to provide an experiential portion to our undergraduate physics program with an educational focus on HPC-specific computing skills, AMO physics, and modern quantum chemistry methods. DFT functionals from the B3LYP, PBE, TPSS, M06, and M11 families with standard Correlation Consistent, 6-311G split valence family, as well as Sadlej, and Sapporo polarized triple-ζ basis sets are being assessed. The GAUSSIAN16 suite on DoD-HPCs is used for quantum chemistry calculations. Our Renner coefficients are compared with previously published theoretical and experimental results to assess the accuracy of various functional/basis set combinations. How method choice affects accuracy will be characterized. An update on the progress of this work will be given at the meeting. Early work on other linear triatomics will also be presented.

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