The Low-Lying Electronic States of NO_2: Potential Energy and Dipole Surfaces, Bound States, and Electronic Absorption Spectrum

Richard Dawes[1], Ernesto Quintas-Sánchez[1], Steve Ndengué[2], David Osborn[3]

1 Missouri University of Science and Technology, Rolla, Missouri 65409, USA
2 ICTP-East African Institute for Fundamental Research, University of Rwanda, Kigali, Rwanda
3 Combustion Research Facility, Sandia National Laboratories, Livermore, California 94551, USA

This talk will provide an extended discussion of a recent paper with the same title (*J. Phys. Chem. A* 2021, **125**, 25, 5519), focusing on the electronic structure and absorption spectrum of NO_2. Some (gory) details and illustrations of the electronic structure protocol and diabatization approach will be given. Going beyond the paper, results will be presented for computed spectra at elevated temperatures, exploring the effects of rotational excitation as high as J=25 and weighted contributions from the lowest 175 vibrational levels.