AB INITIO CALCULATIONS OF VIBRATIONAL LEVELS AND FRANCK-CONDON FACTORS FOR LASER-COOLABLE MOLECULES

CHAOQUN ZHANG, LAN CHENG, *Department of Chemistry, Johns Hopkins University, Baltimore, MD, USA*.

Vibrational energy levels and Franck-Condon factors (FCFs) of laser-coolable molecules has attracted more and more attention because of their promising applications in quantum information science and search for fundamental physics. This presentation focuses on the calculations of vibrational energy levels and FCFs for SrOH and YbOH molecules, which play significant roles in the research of laser cooling. We calculated potential energy surfaces (PESs) for low-lying electronic states of these molecules using scalar relativistic equation-of-motion coupled-cluster (EOM-CC) methods[1]. A standard discrete variable representation (DVR) method[2,3] was then adopted for computations of vibrational energy levels, wave-functions, and FCFs. The accuracy of the calculations was critically analyzed by comparing computational results with experiments[4,5].

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