CALCULATION OF FRANCK CONDON FACTORS FOR METAL-CONTAINING DIATOMIC MOLECULES OF INTEREST TO LASER COOLING USING COUPLED-CLUSTER TECHNIQUES

HANNAH KORSLUND, LAN CHENG, *Department of Chemistry, Johns Hopkins University, Baltimore, MD, USA*; NIKESH S. DATTANI, *Harvard-Smithsonian Center, Harvard University, Boston, USA*.

Franck Condon factors (FCFs) among low-lying electronic states of a molecule are of paramount importance in the study of laser cooling based on optical cycles. The accurate calculation of potential energy surfaces for these electronic states is key to obtaining accurate FCFs. Multireference configuration interaction as a standard approach for computing potential energy surfaces has been the method of choice in many applications. Since the laser cooling procedure focuses on the low-lying vibrational states, only the local potential energy surfaces, for which the multi-reference character is often not pronounced and it is the treatment of dynamic correlation that determines the accuracy of the calculation, are relevant. Therefore, we advocate the use of coupled-cluster (CC) techniques, which provide systematic treatments of dynamic electron correlation, to obtain accurate computational results for FCFs. The yttrium oxide molecule that is subject to active experimental studies [1-3] is adopted here as an example to demonstrate the accuracy of the FCFs using CC potential energy surfaces.

References

[1] M. T. Hummon, M. Yeo, B. K. Stuhl, A. L. Collopy, Y. Xia, and J. Ye, Phys. Rev. Lett. **110**, 143001 (2013).

[2] A. L. Collopy, M. T. Hummon, M. Yeo, B. Yan, J. Ye, New J. Phys. **17**, 055008 (2015).

[3] A. L. Collopy, S. Ding, Y. Wu, lan A. Finneran, L. Anderegg, B. L. Augenbraun, J. M. Doyle, and J. Ye, Phys. Rev. Lett. **121**, 213201 (2018).