Missouri S&T Chemistry Seminar

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Theoretical study of long-range molecular interactions

Abstract

The study of intermolecular forces is essential for predicting and understanding the dynamics of molecular systems, which can be relevant to numerous scientific disciplines, including atmospheric chemistry, environmental chemistry, and astrochemistry. Recent discoveries of complex organic and especially chiral molecules in the interstellar medium have drawn a lot of interest, and theory and simulation are important partners to experimental measurements in these efforts. Interactions between molecules in the gas phase can be separated into short- or long-range forces, depending on whether their molecular electronic clouds overlap. For modelling purposes, these interactions can be better understood and represented by constructing a potential energy surface (PES) for the system of interest. In this talk, some methods and applications of fitting PESs will be discussed, with particular focus on a new framework for treating the long-range region. A software package "Long-Range-Fit" (LRF) was developed, implementing a physically rigorous description of interactions in the long-range region, namely electrostatic, induction, and dispersion. An interactive user-friendly interface connects the user to the underlying sophisticated high-order mathematical treatment.