The central role of the potential in reaction dynamics and energy transfer

Joel M. Bowman Cherry L. Emerson Center for Scientific Computation and Department of Chemistry Emory University, Atlanta, GA USA 30322

Abstract

My group has developed many high-dimensional potential energy surfaces (PESs) using permutationally invariant fitting of tens to 100s of thousands of electronic energies, most often at the CCSD(T) level of theory. These range from PESs that describe non-reactive systems, most recently H_2+CO for low-energy quantum scattering applications, and CH_4+H_2O, and $CH_4(H2O)_2$ for energy transfer and clathrates to recent reactive systems such the unimolecular dissociation of CH_3OH to numerous products and the unimolecular dissociation of syn-CH_3CHOO to OH plus vinoxy. My talk will briefly review the techniques we have developed to obtain PESs (and also dipole moment surfaces) and then selected results from recent applications will be given. The names and photos of the many group members involved in this work will be given

Financial support from the National Science Foundation, Department of Energy, Army Research Office and NASA is gratefully acknowledged.

Solvay Workshop on Atomic and molecular collision mechanisms