Overview Talk on Potential Energy Surfaces

Joel M. Bowman, Bastiaan J. Braams, Yimin Wang

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

The currently exists a variety of methods to represent potential energy surfaces for high dimensional systems, and these will be reviewed after a short, selective, historical introduction to the topic. I will describe the progress we have made. The central aspect of progress is to perform standard least-squares fits of the order of 10^4 "scattered" electronic energies using a polynomial basis that is invariant with respect to all permutations of like atoms. Some of the technical details of this approach will be given followed by several case studies with a focus on recent work on the water dimer and trimer.

I will conclude with a review of some related fitting strategies, which are quite different from full-dimensional fitting approaches, which are know as "n-mode representation of the potential", the "high dimensional model representation" and the "potfit".

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