COMPUTATIONAL MODELLING IN THE 21ST CENTURY

EDWARD F. HAYES, *Department of Chemistry, The Ohio State University, Columbus, OH-43210*.

Computational chemists today are able to achieve about 10 Gigaflops sustained performance on massively parallel processor (MPP) architecture machines for a number of spectroscopic applications. Over the next few years, commercially available computer systems – available to chemists for routine studies – are likely to increase the sustained performance levels a thousand fold to levels exceeding 10 Teraflops. What are the implications of this growth in computing capability for spectroscopists and computational chemists? A few possible developments will be discussed based on extrapolations from current work at The Ohio State University. These will include examination of the prospects of moving from full quantum treatments of the rovibrational spectrum of three atom systems to four, five and six atom systems, examination of even more complex systems using reduced dimensional methods, as well as examination of better functional forms for potential energy surfaces and improved nonlinear optimization strategies for matching to experimental data. Prospects for achieving even greater computational capability as a result of improvements in grid methods, selection of optimal coordinates, and new MPP approaches (such as to obtaining eigen solutions, to solving linear equations, and to accelerating nonlinear optimization fits) will also be discussed. Finally, the implications of these developments for molecular electronic structure studies will be analyzed.