COMPUTATIONAL CHEMISTRY

Although some may have envisioned it, most people in the field did not fully foresee the impact computers would have on chemistry. Before the late 1950s and early 1960s, the time when digital computers became available to scientists, the theoretical underpinnings of chemistry were based on analytically solvable models. By their simplistic necessities, the models often provided incomplete and at best only qualitative representations of molecules and collections of molecules. Standard paradigms for the models included separable degrees of freedom (whether motions of electrons or vibrations and rotations of nuclei) and statistical populations of energy levels. Including the actual nonlinear couplings of electronic and nuclear motions along with the time-dependence of energy-level populations was not possible.

With access to digital computers, chemists quickly investigated the properties of more complete theoretical models. Their approaches were both deductive in performing more accurate calculations for accepted models and inductive in using computers to treat complex molecular systems and in testing the fundamental assumptions of theoretical models. Performing experiments on computers and in the laboratory are now possible.

Scientists performed pioneering computational chemistry studies in the fields of statistical mechanics, chemical dynamics, and quantum

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chemistry, fields that at the time were quite disparate. In 1950, Boys proposed the use of Gaussian orbitals in computational quantum chemistry, circumvecting the main obstacle that molecular wavefunction calculations had suffered since the discovery of Schrödinger's equation in 1926. In 1957, Alder and Wainwright reported the first molecular dynamics simulation, which investigated the solid–liquid phase diagram of a hard sphere system. Bunker reported a trajectory study of triatomic dissociation in 1962, comparing the simulation results with the predictions of statistical unimolecular rate theory. The importance of these pioneering works and the ensuing advances in computational chemistry was highlighted by the 1998 Nobel Prize awarded to John Pople for his research in computational quantum chemistry and the inception and early development of the widely used Gaussian computer program.

To prepare this special issue, we asked several experts to write articles emphasizing current advances in computational chemistry. These articles illustrate the exciting opportunities for computational chemistry, in both the complexity of the systems that we can investigate as well as the accuracy that we can obtain. They also show how computation has helped integrate fields of chemistry and blur the boundaries between statistical mechanics, chemical dynamics, and quantum chemistry. We hope you enjoy reading these articles, and we welcome your thoughts regarding the future of computational chemistry.

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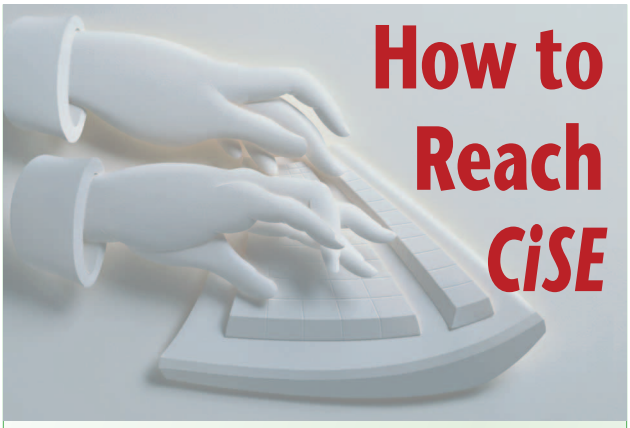

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