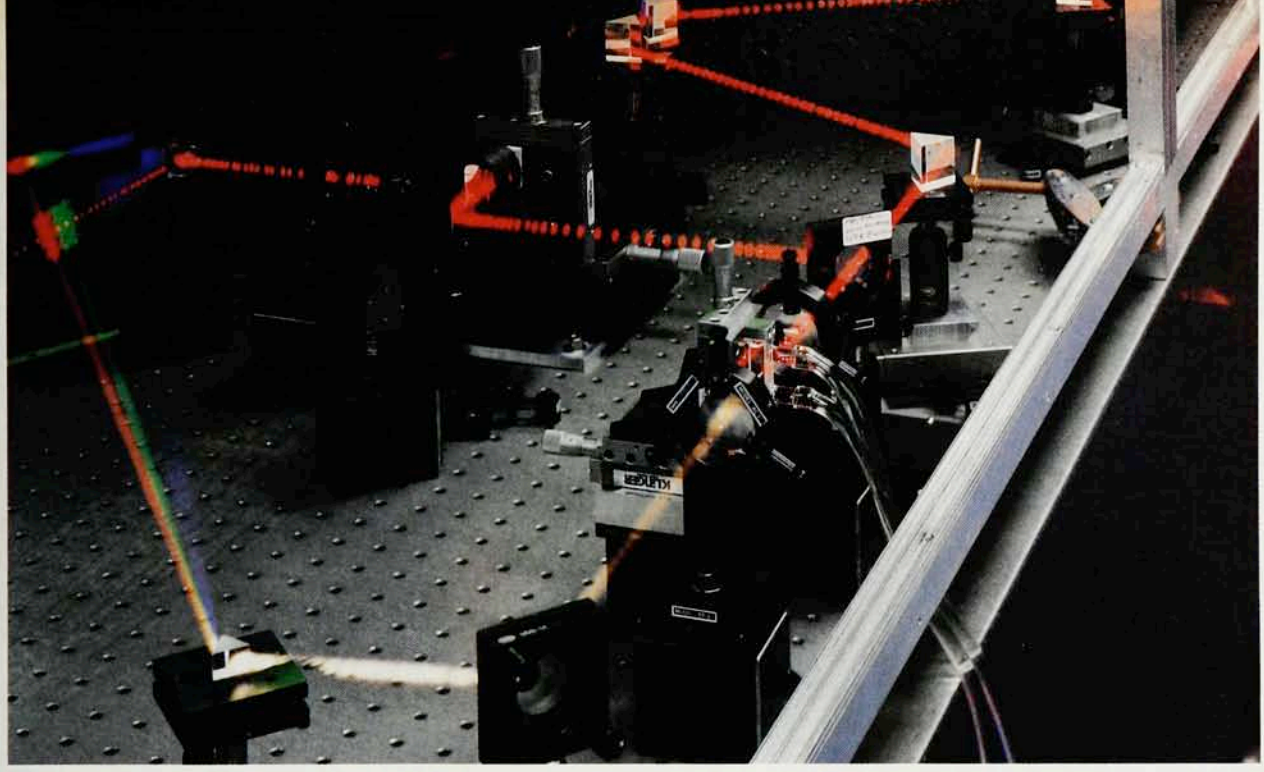

Ultrafast lasers are the key to studying molecular dynamics. (Caltech photo.)

SPECIAL ISSUE:

DYNAMICS OF MOLECULAR SYSTEMS

The development of ultrashort light pulses during the last decade has opened the way to the direct probing of the fundamental dynamic processes of molecular systems. Coupled with the huge strides made in handling complex, many-body systems by computer simulation and the continued development of molecular theories, the availability of these ultrashort lased pulses has allowed our understanding of reaction dynamics and their subtleties to flourish. Our goal is to achieve a high level of predictability concerning the dynamic behavior of molecular systems in a broad range of disordered environments. However, the individual approaches to this goal—that is, the ways in which the fundamental scientific issues of molecular dynamics are studied—have varied.

Current views of molecular dynamics as it relates to chemical reactions and molecular transport are based on an extensive body of work, beyond the scope of this special issue. What we offer here is an overview of some of recent theoretical and experimental studies that have contributed to our overall knowledge. Each article addresses the theme of dynamics of molecular systems in a different chemical environment. Molecular disorder is the common element uniting all of the chemical systems studied. (The reader can gain a perspective of the time scale of the dynamic processes covered in this issue from figure 2 in the article on page 36.)

Martin Gruebele and Ahmed H. Zewail focus on gas-phase molecular-beam ultrafast reaction dynamics in their article on page 24. The authors provide examples of chemical reactions that can be studied on a fundamental chemical time scale from 10 femtoseconds to 10 picoseconds. In doing so, they emphasize the importance of the transition state in chemical reactions.

Graham R. Fleming and Peter G. Wolynes, in the article on page 36, consider chemical dynamics in liquids. They review solution-phase chemical reactions and recent developments in experimental techiques, theory and computer simulations. In particular, they cover four phenomena that influence the dynamics of solutions: friction, activated processes (for which the applicability of the transition state in liquid reactions is considered), dynamics and electron-transfer reactions.

In our article on page 46 we consider the dynamics of both gas- and liquid-phase molecular systems that are confined to the microenvironment of a porous glass. Recent studies connect the size of the confining space to the dynamic and thermodynamic behaviors of the molecular systems.

In the article on page 58, Dieter Haarer and Robert Silbey discuss the two-photon spectroscopy of hole burning for molecules dissolved in glasses. These authors illustrate the relationship between the magnitude of the homogeneous linewidth and its temperature dependence in the host glass by considering the structural and dynamical properties of glassy states.

We hope that the package of articles in this issue will provide some understanding of the corroborative efforts among researchers in molecular dynamics. The articles are but snapshots of a field where ongoing developments in lasers and computers are leading to new results and to new perceptions among theorists and experimentalists.

J. M. Drake
Exxon Research And Engineering Co
J. Klafter
Tel Aviv University ■