

JCTC

Journal of Chemical Theory and Computation

Introducing the *Journal of Chemical Theory and Computation*

Welcome to the *Journal of Chemical Theory and Computation (JCTC)*. This new American Chemical Society journal is being introduced to provide a focal point for publication of articles, letters, and reviews reporting new theories based on physical laws, advances in computational methods, and important applications to problems in chemistry. Though the contents will evolve, some specific topics that are appropriate today for *JCTC* include advances in or applications of ab initio quantum mechanics, density functional theory, statistical mechanics, design and properties of new materials, surface science, Monte Carlo simulations, solvation models, QM/MM calculations, biomolecular structure prediction, and molecular dynamics in the broadest sense including gas-phase dynamics, ab initio dynamics, biomolecular dynamics, and protein folding.

Many theoretical and computational chemists have believed for a long time that their rapidly expanding community should be represented in a dedicated ACS journal. Their work is currently dispersed over a wide variety of journals in which they often represent a minority interest. The ACS has now responded, and you are invited to participate in this undertaking to establish *JCTC* as the central source for the best work in the field. The ACS connection will provide reassurance that all aspects of the processing of manuscripts will be handled professionally and efficiently and that the resultant publications will benefit from state-of-the-art appearance and worldwide accessibility. To facilitate this, manuscript submission and review for *JCTC* will only occur through the online ACS Paragon System. The Journal is off to a great start as documented in this first issue. It is hoped that the birth of *JCTC* will be viewed in time as a notable event comparable to the introduction of predecessors such as the *Journal of Physical Chemistry* in 1896 or the *Journal of Chemical Physics* in 1933. In the latter's first issue, its editor, Harold Urey, observed: "The life and interests of the individual are short and of little consequence as compared to the lives of our sciences." This will always be true, and our only intention is for *JCTC* to help enrich the science through improved publication and sense of community.

There are many people who deserve thanks for bringing *JCTC* to fruition. The support, encouragement, and handling of innumerable details by the ACS Board of Directors, Executive Director & CEO Madeleine Jacobs, President of the ACS Publications Division Robert Bovenschulte, Vice President for the Journal Publishing Group Mary Scanlan, their endlessly helpful staffs, the Editorial Advisory Board, and Editorial Assistant Patricia Morales have been essential.

William L. Jorgensen
Editor

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