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Journal Interviews : 2009 : Journal of Chemical Theory and Computation

JOURNAL INTERVIEWS - 2009

June 2009



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Journal of Chemical Theory and Computation

A Featured Journal from *Essential Science Indicators*SM

Late last year, Essential Science Indicators from *Thomson Reuters* named the Journal of Chemical Theory and Computation (JCTC) a *Rising Star* in the field of Chemistry for the period of April to June 2008. The journal's current citation record includes 743 papers cited a total of 4,965 times from its inauguration in 2005 to February 28, 2009.

JCTC is one of the many journals published by the American Chemical Society. The journal's aim is "Reporting new theories, methodology, and/or important applications in quantum chemistry, molecular dynamics, and statistical mechanics." The co-editors of JCTC are Prof. William Jorgensen of Yale University and Prof. Gustavo Scuseria of Rice University.

In the interview below, ScienceWatch.com talks with Professors Jorgensen and Scuseria, as well as Sarah Tegen, the Assistant Director for Editorial Development, about the journal's history and citation record.

SW: Did you expect the *Journal of Chemical Theory and Computation* to become highly cited, or is this surprising to you?

JCTC is one of more than 30 journals published by the American Chemical Society, many of which are leaders in their respective disciplines. We have high expectations for all of our journals, so the only surprising aspect for JCTC is that it has become such a highly cited journal after only four years of publication. JCTC filled a niche in our portfolio; theory and computation was found in many journals (and still is) but there was no dedicated home for these articles.

SW: How would you account for the high citation rate of JCTC?

The editorial team for JCTC strives to publish the best articles submitted to the journal. Of course, the high citation rate is also because our authors submit high-quality research articles to the journal, and our network of peer-reviewers helps further improve the submitted papers. Additionally, having a journal exclusively dedicated to theoretical and computational chemistry has helped broadened the audience and the impact of this field.

SW: Would you give us a brief history of the journal?

JCTC was launched in 2005 as a bimonthly publication with Prof. William Jorgensen (Yale University) as the editor. One-hundred and thirty-three articles were published in the inaugural volume. In 2008, the journal expanded to 12 issues per year, published 219 articles, and added Prof. Ursula Rothlisberger (Swiss Federal Institute of

Technology) as an associate editor. 2009 saw a further expansion of the editorial team, with Prof. Gustavo Scuseria (Rice University) coming on board as co-editor with Prof. Jorgensen. Prof. Jorgensen and Prof. Scuseria are both ISIHighlyCited researchers.

SW: What historical factors have contributed to the success of JCTC?

JCTC is a young journal, so its history is brief. However, success can be attributed to its focus on publishing the most appropriate articles, through the enforcement of high editorial standards, rapid processing times, and cultivation of a distinguished advisory board.

SW: Have there been specific developments in the fields served by JCTC that may have contributed?

In addition to the excellent articles submitted by authors, computational and theoretical chemistry are growing areas of chemistry. We have also observed that thematic and special issues are very popular with our readership. By maintaining selectivity in a growing field, we help ensure the success of JCTC.

SW: What, in your view, is this journal's main significance or contribution in the field of Chemistry?

JCTC has been clearly welcomed by the theoretical and computational chemistry community. It serves as a natural home for those authors publishing work related to biomolecular systems, condensed phase theory, dynamics, electronic structure, and quantum chemistry, among others.

SW: How do you see your field(s) evolving in the next few years?

Theory and computation is bound to have a large impact on science going forward. Faster computers, better algorithms, and more accurate methods will all contribute to the continuing partnership between theory and experiment.

SW: What role do you see for your journal?

We foresee JCTC continuing down the path of publishing the best material in computational and theoretical chemistry. The continued focus will be on quality, not quantity, of articles. We expect JCTC will be a leader in the publication of existing and emerging fields in the always-evolving theory and computation landscape. ■

Journal of Chemical Theory and Computation

William Jorgensen, Ph.D., co-Editor

Gustavo Scuseria, Ph.D., co-Editor

Sarah Tegen, Ph.D., Assistant Director, Editorial Development

American Chemical Society, publishers

Journal of Chemical Theory and Computation's current most-cited paper in Essential Science Indicators, with 186 cites:

Zhao Y, Schultz NE, Truhlar DG, "Design of density functionals by combining the method of constraint satisfaction with parametrization for thermochemistry, thermochemical kinetics, and noncovalent interactions," *J. Chem. Theory Comput.* 2(2): 364-82, March-April 2006. Source: *Essential Science Indicators* from Thomson Reuters.

Additional Information:

- William Jorgensen and Gustavo Scuseria are featured in ISIHighlyCited.com

KEYWORDS: AMERICAN CHEMICAL SOCIETY, THEORETICAL CHEMISTRY, COMPUTATIONAL CHEMISTRY, NICHE JOURNAL, BIOMOLECULAR SYSTEMS, CONDENSED PHASE THEORY, DYNAMICS, ELECTRONIC STRUCTURE, QUANTUM CHEMISTRY, THEMATIC ISSUES.



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