Chelli, J Theor Comput Sci 2013, 1:1
DOI: 10.4172/2376-130X.1000e102

Journal of
Theoretical & Computational Science

Editorial Open Access

Journal of Theoretical and Computational Science: Open Access, A Bridge to Link Knowledge from Chemistry, Physics, Biology and More

Riccardo Chelli[1,2]*

[1]*Dipartimento di Chimica, Universita` di Firenze, Via della Lastruccia 3, I-50019 Sesto Fiorentino, Italy and*
[2]*European Laboratory for Non-linear Spectroscopy (LENS), Via Nello Carrara 1, I-50019 Sesto Fiorentino, Italy*

Welcome to the Journal of Theoretical and Computational Science: Open Access (JTCO). This new open access journal is being introduced to provide a focal point for publication of articles, letters, and reviews (see Ref. [1] for detailed information about publication formats) reporting advances in chemical and physico-chemical theories, computational methods, and important applications to problems in chemistry, physics and biology. The Journal will also dedicate special attention to computational aspects of biomedical sciences, including pharmaceutics, bioinformatics and drug discovery. Applications of high performance computing to the scientific advancement and human therapeutics will be object of publication as well. Though the contents will evolve, some specific topics in the chemical and physical frameworks that are appropriate today for JTCO 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. No less important is the intention of attracting audience from diverse other fields which traditionally are not part of the orthodoxy of theoretical and computational sciences. These fields include software development, information science, network theory, chemical informatics, clinical informatics, medicinal chemistry, bioinformatics, computational neuroscience, synthetic biology, and toxicology (additional information about the fields of interest to JTCO can be found in Ref. [1]).

Such a variety of research fields will allow to make a bridge between scientists with very different background, facilitating the exchange of knowledge between worlds that, still today, have several problems of communication. To this aim, the Reviewers will be asked to put special attention to the language employed by the authors, which should not be too technical in order to reach a broader readership. This does not mean that technical articles will be discouraged, but that additional paragraphs or sections may be required to the authors to present the basic aspects of the research in a simpler fashion. Thus, the strongly multidisciplinary character of JTCO has the ambition of creating a link between those theoretical and/or computational scientists that often limit their publishing activity to specialized journals. In addition to the aim of creating a network between researchers of the "world wide web" of technological sciences, JTCO is also a space where theoretical reports, in the sense of pen & paper products, can find worldwide visibility, comparable to computational studies.

However, we must acknowledge that this challenging target is common, at least in part, to several journals, starting from the popular Journal of Chemical Theory and Computation published by the American Chemical Society. So, what are the most relevant differences between JTCO and the other journals, especially the other open access journals? In my opinion, they can be summarized with three keywords: transparency in peer reviewing, stimulation of the scientific debate, acknowledgment of the quality of the research.

Transparency in peer reviewing: At variance with all other journals, the Reviewers' names will be provided as supplementary information to the publication (upon decision of the Editor and acceptance of Reviewers themselves). This will make the Reviewers not only aware of their responsibilities in front of the scientific community, but will also give the due appreciation to their hidden work. Moreover, upon Editor's decision and Authors' acceptance, negative or particularly critical peer reviews could be published together with the article (with no charges for Reviewer) and will be classified as Opinion Article.

Scientific debate: Considering that the evaluation of an article is in large part left to the peer reviewing process and that, rarely, articles with wrong data, unclear methods, or simply with questionable conclusions are retracted or, at least, object of comments by the scientific community, JTCO encourages the scientific debate by publishing Comments to Articles with no charges.

Quality of the research: In order to reward the high quality research, outstanding research articles, reviews, etc. will be published in JTCO with no charges.

The Editorial staff 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. It is hoped that the birth of JTCO will be viewed in time as an event comparable to the introduction of predecessors such as the Journal of Chemical Theory and Computation in 2005 or the Journal of Computational Chemistry in 1980.

References

1. Dakshanamurthy S (2013) Editorial Policy: Journal of Theoretical & Computational Science: Open Access. J Theor Comput Sci 1: 1-1.

***Corresponding author:** Riccardo Chelli, Dipartimento di Chimica, Universita` di Firenze, Via della Lastruccia 3, I-50019 Sesto Fiorentino, Italy and European Laboratory for Non-linear Spectroscopy (LENS), Via Nello Carrara 1, I-50019 Sesto Fiorentino, Italy, Tel: +39-0554573082, E-mail: riccardo.chelli@unifi.it

Received August 21, 2013; **Accepted** August 21, 2013; **Published** August 28, 2013

Citation: Chelli R (2013) Journal of Theoretical and Computational Science: Open Access, A Bridge to Link Knowledge from Chemistry, Physics, Biology and More. J Theor Comput Sci 1: e102. doi: 10.4172/2376-130X.1000e102