



Inaugural Editorial

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The universe of computational and theoretical chemistry is rich, vast, and growing exponentially. The major impetus behind this extraordinary growth curve in recent decades has undoubtedly been the profusion of scientific and technological breakthroughs. Arbitrarily choosing my lifetime (1950-) as a yardstick, we have witnessed an almost endless progression of amazing scientific discoveries and technological achievements: the discovery of DNA's structure and, thereupon, the birth of molecular genetics in the 1950s; the Space Age in the 1960s and 70s; the Digital Age and rise of the personal computer in the 1980s; the emergence of the supercomputer, the Internet, and the World Wide Web in the 1990s; the outgrowth of genomics and bioinformatics from the Human Genome Project in the 2000s; to the Information Age (Informatics) today. Individually and together, these scientific and technological advances, and many others omitted here for the sake of brevity, have forever transformed the landscape of theoretical and computational science. We have every reason to expect that the procession of scientific and technological discoveries, inventions, and innovations will continue into the future. In each of these developments, theoretical and computational science has played the role of both benefactor and beneficiary. Truly, there is no time riper than the present to launch an open access journal for scientists who are active in the development and application of theoretical and computational chemistry and related fields of study. This personal assessment is stated in full knowledge of the hardships caused by the current economic downturn, which hopefully is a temporary blip. It is within this optimistic and reflective context that we are delighted to welcome authors and readers to this inaugural issue of the *Journal of Theoretical and Computational Science: Open Access*.

Pondering the chronology of the scientific leaps cited above, it is fair to assert that we exist in a new Golden Age of scientific and technological developments. As a practitioner in theoretical and computational chemistry for the past 40 years, I must confess to a lack of appreciation of this seemingly obvious realization. Two explanations for my mental block come to mind. First, the coinage of each major discovery as an "Age" (as in Digital Age) or "Revolution" (as in Genomic Revolution) has tended to obscure the clear evidence of mutual interdependence within this sequence of eventful scientific discoveries. Perhaps aside from the Space program that was motivated largely by political ideology, each discovery appears to be a direct evolutionary descendant of the preceding discoveries. The final destination of this pathway of scientific discovery is hard to discern, but it is unlikely to occur anytime soon. It is certain, however, that theoretical and computational science will play a vital role throughout and beyond. Second, the rapid pace, immediacy, and familiarity of these scientific advances have instilled in us the impression that these discoveries are self-sustainable. Only upon stepping back does one recognize that the present Golden Age is indebted to seminal contributions by theoretical and computational science. Likewise, each of these innovative accomplishments offers tangible proof of the utility and versatility of theoretical and computational science. A short list of the relevant fields that contributed to, and evolved from, the proliferation of historic events during this new Golden Age includes molecular modeling & simulation; high performance computing; pattern recognition, machine learning, and optimization methods; computer science, information

technology, and algorithmic development; materials design and nanotechnology; quantum mechanics and dynamics; bioinformatics, cheminformatics, and clinical informatics; computational & systems biology, rational drug design, and predictive toxicology. The Journal invites contributions from the broad expanse of these diverse fields.

From the perspective of this editorial, it is a momentous time to launch the *Journal of Theoretical and Computational Chemistry: Open Access*. Accessibility via the internet will expedite the review, publication, and dissemination of manuscripts, thereby offering speed and convenience to authors, reviewers and readers. The Journal's editorial policy will ensure an open forum for scientists to interact with each other, express and exchange ideas, introduce new concepts at the interfaces of established disciplines, and thereby expand research horizons. The open access of the Journal is especially attractive for young scientists, whether theoretician or experimentalist, to gain free access to the latest developments in the multifaceted realm of theoretical and computational science. In conclusion, it is anticipated that authors and readers of the Journal will find ample opportunities for insight, discovery, and innovation. Welcome to the Journal!

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Received September 04, 2013; Accepted September 06, 2013; Published September 16, 2013

Citation: Welsh WJ (2013) Inaugural Editorial. J Theor Comput Sci 1: e104. doi: 10.4172/2376-130X.1000e104

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