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Advantages and Requirements of Growing Theoretical and Computation Research and Dissemination of Results in Open Access Journals

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Even without touching any chemical, the chemistry of a wide range of systems, starting from simple molecules to complicated biologically relevant molecules to nanomaterials, can be studied and several underlying chemical features can be understood using Theoretical and Computation methods. Theoretical and computational investigations are complementary and supportive to experimental studies, and became essential tools in modern high-end research. These tools are instrumental in understanding simple to complex chemical processes, complex structures and their reactivity. Besides these features, designing new materials by modeling, revealing new properties and on how to tune relevant properties in desired directions for application-oriented products has become a key application of theoretical and computational chemistry research in present days.

Theoretical and computational research does not require expensive and high-end instruments, such as high resolution microscopes besides simple to sophisticated analytical tools. It requires only a single tool i.e., a computer and that is the most advantageous in conducting theoretical research over experimental research. Rapid advancement of computer hardware over last two to three decades, and affordability of small to mid-range computers, personal computer (PC) to cluster of computers, enhanced theoretical research activities exponentially in recent years. For example, today's PC with multi-processors or multi-cores, 4-8GB memory with a couple of terabyte (TB) hard disks is almost equivalently efficient in computational calculations to 30-40 years back mid-range high-performance computers.

The second key component of theoretical and computational research is the program codes based on Molecular Mechanics, Quantum Mechanics and Statistical Mechanics, and over the years several research groups developed related programs codes, and some of those codes are available freely. With the development of computer hardware, especial emphasis is given in recent years to developing and making those codes to be more efficient in using parallel computing. The rapid progress and affordability of both essential components, theoretical and computational research activities has enhanced exponentially world-wide over the last couple of decades.

In general, a major section of theoretical and computational chemistry research is based on applications of theoretical models and methods, such as ab initio, density functional theory (DFT), Monte Carlo method etc. However, another important front is the development of theoretical methods to estimate properties, increase accuracy level, made programs more efficient for larger molecular systems. Several groups are engaged in such development and implementing those mathematical methods in programming codes.

Another key issue related to research is the development of vast databases on biomolecules, crystal structures, materials, drug discovery etc. to disseminate findings worldwide. Based on research area and topics, those databases are named BioInformatics, ChemInformatics and so on. Information technology and computer science helped in organizing and mining those huge data easily and made information handy, regardless of where one lives.

Technological developments, easy access of information and scholarly communication helped growing scientific research activities and events worldwide and that is reflected in the growth of research publications [1]. To accommodate growing research findings, new journals have been launched periodically over the years, and some of those are very specialized and others mostly based on a particular research area. However, several reputed scientific journals required subscription and hence were not accessible to worldwide scientific community. Open access scientific journals are gaining popularity due to free availability of research articles by anyone and also from any corner of the world.

OMICS Publishing Group (www.omicsonline.org) starting a new open access journal based on Theoretical and Computational Science, where research articles on all sectors of the research field, described above and mentioned in Editorial Policy [2] will be published. We hope to make this open access journal as one-stop center for all stakeholders in this field of research. Articles in different forms [2] (such as reviews, short communications, research articles, news and views etc.) directly and indirectly involving theoretical and computational chemistry based research findings, modeling and simulation, development of theoretical tools and algorithm, information based database will be accepted for publication after thorough evaluation.

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