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Editorial

Computational Chemistry in Asia

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Asian civilizations are known for their contributions to science and technology. Modern history has witnessed Japan as a remarkable contributor. China and India have emerged in recent decades as driving leading players. Other Asian nations, such as South Korea, Singapore, Malaysia, and Indonesia, have been investing strongly in research and development as well. As one of the key fields in science, computational chemistry has displayed a similar landscape in Asia. For example, Japanese chemist Kenichi Fukui was the first Asian to be awarded the Nobel Prize in Chemistry in 1981 for his work on the development of frontier molecular orbital theory. Chinese theoretical chemist Aoqing Tang led the development of quantum chemistry in the late 20th Century, which became a major research field in China. Deeply rooted in quantum theory, theoretical/computational chemistry in Asia has branched out and diversified into a wide range of subfields, from those associated with traditional organic, inorganic, analytical, physical, and biological chemistries, to new focuses on the environment, energy, materials, and drug discovery. Particularly, the rapid advance in computer power, the availability of powerful artificial intelligence (AI) algorithms, and the fast accumulation of molecular data have paved the road to the exponential growth of chemical information and modeling. In recent decades, there has been enormous multicentered networking among computational chemists and institutions in Asia. To foster collaborations and deepen knowledge exchanges in the Asian computational chemistry community and outreach to biophysical, mathematical, and computer science communities, we introduce a collection of 26 papers selected from nearly 130 submissions. Geographically, the papers in this collection were submitted from many Asian countries, including China, India, Vietnam, Indonesia, and Singapore. There were also collaborative research papers contributed by authors from Asian and non-Asian countries, such as China-Canada, Vietnam-New Zealand, Singapore-New Zealand, etc. We hope that these articles represent the latest progress in computational chemistry in Asia.

The construction of new methods and algorithms remains the key focus of computational chemistry. In this collection, a variety of papers were devoted to the development of new computational methods or effective algorithms that may significantly enrich the fields of computational chemistry. Specifically, Nguyen et al.[1] constructed an ensemble framework to identify the natural products of anticancer activity. A deep learning-based method was proposed by Krishnan et al.[2] to design target-specific ligands. Nguyen-Vo et al.[3] designed a framework to integrate multitask learning and encoding strategy for screening CYP inhibitors. A molecular encoding scheme was discussed by Nguyen-Vo et al.[4] for accelerating the identification of antimalarial natural products. Huang et al.[5] built a drug-network-screening approach to identify new drug combinations; Li et al.[6] set forward a multimodal deep learning method to compute noncovalent interaction. Finally, a purely graph-based aromaticity indicator and a three-dimensional (3D) CNN-based algorithm were introduced by Wang et al.[7] and Aggarwal et al.[8] to describe molecular physical, chemical, and structural properties.

Besides new method development, other focuses of modern computation chemistry include the successful adoption and application of appropriate methods to solve long-standing problems in the chemical sciences. In this collection, the application of computational methods was aimed at research on *molecular mechanism*, *drug discovery*, and *material/probe design*.

Various molecular dynamics (MD) simulations were carried out in the studies of *molecular mechanism*. For example, Hao et al.[9] used a large-scale MD simulation to thoroughly explore the mechanism underlying the regulation of CETP. MD simulations were adopted by Wang et al.[10] to investigate the intriguing role of glycans in TLR3. Li et al.[11] performed extensive MD studies to delineate molecular details of calcium-induced allostery. A cosolvent MD method was employed by Feng et al.[12] to detect potential binding sites on the surface of BAX. Chen et al.[13] used a randomly accelerated MD algorithm and funnel meta-dynamic simulations to explore the dissociation mechanisms of nonsteroidal GR ligands. *Gaussian* accelerated MD simulations were coupled with a dynamic network to probe the mechanisms of distinct biased activation induced by structural variations by Chen et al.[14] Zhang et al.[15] applied microsecond accelerated MD simulations coupled with a protein structure network to explore allosteric regulation mechanisms. Moreover, other well-established methods also play an important role in mechanism studies. For example, an enhanced sampling technique was adopted to characterize the new dimerization mechanism underlying phosphorylation regulation by Dong et al.[16]

Drug discovery is another popular topic in this collection. Most studies were based on MD simulations and virtual screening (VS). Zhao et al.[17] integrated VS, homology

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modeling, and in vitro enzymatic activity analysis to identify a new triazinoindole compound as CD39 inhibitor. A ligand-based VS protocol was also employed by Huo et al. to identify new EGFR inhibitors.[18] Molecular modeling was performed to investigate the anticancer activity of some synthetic alpha-mangiferin derivatives as human ER-alpha inhibitors by Mardianingrum et al.[19] A series of all-atom MD simulations were carried out by Paul et al.[20] to identify an indanone-carbamate-based molecule inhibitor for the aggregation of amyloid-beta. In addition, several papers concerned *material/probe design*. For example, the synergistic mechanism between protein and ice crystals was revealed by Cui et al.[21] to discover new antifreeze materials. Finally, a multiple-property machine learning method was proposed by Xu et al.[22] to design new promising functional materials.

The inherent interdisciplinary vocation of computational chemistry encompasses a wide variety of other topics. For example, structural modification strategies were developed by Guo et al.[23] to design the photon excitation fluorescence probes. A database was constructed by Wang et al.[24] to explore the impact of distal mutations on enzyme activities. The remaining papers in this collection were devoted to comprehensive reviews. Hariono et al.[25] reviewed decades of research on computer-aided drug design and discovery in Indonesia, and Xie et al.[26] provided a retrospective on 3D molecular generative models for the *de novo* drug design.

Asian computational chemists have been an active part of the *Journal of Chemical Information and Modeling* (JCIM) community. We hope the contributions showcased in this special issue highlight some of the exciting scientific advances made in Asia and promoted by JCIM.

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Notes

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