Special Issue

Machine Learning in Chemistry

Message from the Guest Editors

In recent years, machine learning has started to revolutionize how chemistry is done, including accelerating the exploration of the chemical compound space, proposing new reaction mechanisms or synthetic pathways, exploring the potential-energy surfaces, and understanding the fundamental quantum mechanical principles of theoretically challenging systems. An enormous amount of machine learning techniques have been developed by computer scientists, data scientists, physicists, and chemists, and they have been widely applied in physical sciences. This dynamic research field has attracted researchers from different disciplines to work together to propose new methods, design new architectures, and unlock creative ways for applications. This Special Issue is devoted to "Machine Learning in Chemistry". It will cover all aspects of using machine learning to investigate reaction mechanisms, molecular structures, catalysts design, material properties, organic synthesis, molecular generation and optimizations, and fundamental electronic-structure calculations.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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