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Editorial on Computational Chemistry

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Editorial

Computational chemistry is a discipline of chemistry that employs computer simulations to aid in the resolution of chemical problems. It calculates the structures and characteristics of molecules and materials using theoretical chemistry methods merged into efficient computer systems. It is required because, with the exception of recent results involving the hydrogen molecular ion (dihydrogen cation; see references for more information), the quantum many-body problem cannot be solved analytically, let alone in closed form. While computational results are typically used to supplement knowledge received through chemical experiments, they can also be used to forecast chemical processes that have yet to be observed. It's employed a lot in the development of novel medications and materials. Both static and dynamic circumstances are covered by the approaches used. With the size of the system being investigated, computer time and other resources (such as memory and disc space) expand significantly. A single molecule, a group of molecules, or a solid can make up that system. The accuracy of computational chemistry methods varies from very approximate to extremely precise; the latter is usually only possible for tiny systems. Quantum mechanics and fundamental physical constants are used exclusively in ab initio procedures. Because they use additional empirical parameters, other approaches are referred to as empirical or semi-empirical.

Approximations are used in both ab initio and semi-empirical techniques. These might range from simplified first-principles equations that are easier or faster to solve, to approximations that limit the size of the system (for example, periodic boundary conditions), to fundamental approximations to the underlying equations that are essential to produce any solution at all. Most ab initio computations, for example, use the Born–Oppenheimer approximation, which considerably simplifies the underlying Schrödinger equation by assuming that the nuclei remain stationary throughout the calculation. As the number of approximations is minimized, ab initio approaches should finally converge to the exact solution of the underlying equations.

However, it is hard to eliminate all approximations in practice, and residual error is unavoidable. The purpose of computational chemistry is to maintain the computations tractable while minimizing residual error.

In some circumstances, the electrical structure of molecules is less relevant than their long-term phase space behavior. In protein conformational research and protein-ligand binding thermodynamics, this is the case. To enable lengthier simulations of molecular dynamics, classical approximations to the potential energy surface are utilized, often with molecular mechanics force fields, because they are computationally less costly than electronic calculations. In addition, cheminformatics employs even more empirical techniques, such as machine learning based on physicochemical features. Predicting the binding affinity of medicinal compounds to a particular target is a common topic in cheminformatics. Predicting binding selectivity, off-target effects, toxicity, and pharmacokinetic features are among the other issues.

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