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Opinion Article

Computational Chemistry is used to Predict Reactivity

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DESCRIPTION

Computational chemistry is a department of chemistry that uses computer simulation to assist in solving complex chemical problems. It exploits techniques of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures, interactions, and properties of molecules. Computational Chemistry (CC) is most important because, apart from relatively recent results concerning the hydrogen molecular ion, the quantum is a body problem cannot be solved analytically, and much less in closed form. While computational chemistry results usually complement the information obtained through a chemical experiment, it can in some cases predict hitherto unobserved chemical phenomena. It is mostly used in the design of new drugs and materials.

Examples of such properties are structure i.e., the expected positions of the constituent atoms, absolute and interaction energies, electronic charge density distributions, dipoles and better multi pole moments, vibrational frequencies, and other spectroscopic quantities for collision with different particles. The duties of a computational chemistry involve by using computers to help perform experiments and research. In a computational chemistry, you use computer theory to make predictions about the results of theoretical analyses of molecules and solids. It is provides insights into how chemical compounds can bind in the active site of a protein to promote its function. These computational tools provide insights into the dynamics of protein motions and can be used to predict what happens when an amino acid is substituted through another one. Research in theoretical and experimental physical chemistry consists of ultrafast study reaction dynamics, photo acoustic, applications of chemical physics to medical imaging, computational and quantum chemistry, and molecular interaction in liquids.

The actual computational chemistry studies deal with problems for which analytical solutions are not possible, for example, the dynamics of a gas. In such cases, we might use theoretical findings to set up a computational model which can be solved numerically; hence it is a numerical study. Professional level computational chemistry may also pursue a teaching and research career in academia work in industry or for a government organization or national laboratory. They may also support and train facility students, or customers develop new capabilities for collecting and analyzing data. The Quantum Mechanics (QM) is deemed the hardest part of physics. Systems with quantum behavior don't follow the rules that we are used to, they are hard to see can have controversial features, exist in different states at the same time and even change depending on whether they are observed. Computational Chemistry (CC) has different aspects: Computational studies, used to find a starting point for a laboratory synthesis understanding experimental data, which includes the position and source of spectroscopic peaks. A computational study is used to predict the possibility of so far entirely unknown molecules and to explore reaction mechanisms not readily studied through experiments.

CONCLUSION

Thus, it can be assist the experimental chemistry can challenge the experimental chemistry to find entirely new chemical objects and different major areas may be distinguished within computational chemistry. There are different techniques suitable in computational chemistry, including Density Functional theory (DFT) techniques. Among those techniques, density functional theory calculations have received an important role in investigating the interactions between BNNTs and drug molecules during the past few years many attempts have been performed to investigate the interactions of BNNTs with various molecules by using this approach. It has now become an integral component of the adsorption technology applied to porous solids. The purpose of this chapter is to focus on how modeling tools are valuable not only to assist but also to guide the experimentalists throughout the characterization of the materials and the determination of their diffusion properties.

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