Brief history of computational chemistry: Three distinct eras and the relative importance of theoretical insights and computing power in advancing the field

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New in this version

Language is improved in this version.

Conflicts of interest

The author declares no conflicts of interest.

Author's contributions

Wenfa Ng read the computational chemistry literature and an idea crystallized in his mind that posits the possible delineation of the history of computational chemistry into different eras. Articulating ideas into prose, he wrote this abstract preprint.

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Abstract

The past influences the present and future; for example, in computational chemistry, simplifying assumptions and approximations important in the pre-computing era remains relevant today in allowing simulation of larger systems with reasonable amount of computer time. By highlighting significant milestones in efforts (theoretical and simulation) aimed at understanding the nature of a chemical bond, a short essay traces the development and evolution of electronic structure calculation methods over the years. Using temporal relationships between methods as guide, placing the various methods along a time line clusters the methods into three distinct eras, each defined by their relative reliance on theory, approximations, experiment data and computing power for problem solution. Specifically, theoretical models built for explaining spectroscopic emission spectra laid the foundation of the field when theory lagged behind experiment. Promulgation of the Schrodinger equation – which describes total system energy and properties from a quantum mechanical perspective - shifted the focus of the field towards developing methods for solving the equation. However, difficulty in solving the Schrodinger equation during the pre-computing era spawned an entire subfield seeking to develop increasingly refined methods for obtaining approximate solutions. Specifically, semi-empirical methods rely on experiment data to supply parameter values inaccessible through direct calculations from first principles, while approximate methods use simplifications to obviate the need for calculating cross interacting terms. Availability of large amount of inexpensive computing power in recent years brought forth *ab initio* (first principles) simulation methods capable of calculating electronic structure properties of large systems (e.g., long chain biomolecules) with few or no simplifying assumptions and at increasingly fine scales. But, high power computational resources are not easily accessible outside of research institutes. Hence, in what is known as coarse-graining, contemporary research focuses on developing methods for simulating, in high resolution, only important aspects of the problem while leaving other areas of the problem definition (simulation model) to coarser techniques. Together, coarse-graining facilitates probing realistic system sizes for answers in sync with reality. The delineated chronological thread also provides the backdrop for asking counterfactual ("what if") questions examining, from a historical vantage point, the relative roles of computing power and theoretical intuition in the evolution of computational chemistry. Contrary to widespread notions that advances in computational chemistry are solely potentiated by increases in computing power, the essay argues that the relationship between theoretical imagination and computing power is more nuanced: specifically, the two exert differing influence at specific junctures in the field's evolution.

Keywords: chemical bonding; modeling; atomic model; Schrodinger equation; approximate solutions; computational speed; intuition; imagination; science history;

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