

What is Electronic Structure Theory?

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Editorial

Computation Chemistry is general term covering any use of computing in the direct study of chemical problems. As such , it includes the entire range of computational techniques that are applied Chemistry, whether their roots lie in physics- eg., quantum mechanics, stastical mechanics-mathematics, informatics and/or other underlying scientific disciplines. Computational chemistry techniques can predict molecular properties for comparison with experiment, to elucidate ambiguous or otherwise unclear experimental data, and to model short-lived, unstable intermediates and transition states which are impossible to observe directly.

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Quantum Chemistry is a more specific term which refers to methods that were derived, in whole or in part, from the basic laws of quantum mechanics, most directly, the Schrödinger equation. Quantum chemistry can be conceptually divided in to two broad areas.

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