Molecular Properties and Interactions: A Wonderful Playground for a Theoretical Chemist

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Our understanding of the electronic structure of molecules often comes from spectroscopic investigations in which electromagnetic radiation is applied to a molecule and the scattering or absorption of the radiation is measured. These experimental techniques probe the structure and properties of molecules by observing their response to applied electromagnetic perturbations. Such measurements provide a detailed picture of molecular systems, often rich in detail and sometimes difficult to interpret.
Molecular electronic-structure theory has developed to a stage where it can be used to investigate a large number of molecular properties of increasing complexity, with control over the accuracy of the results, and provide invaluable help in the interpretation of experimental measurements of a broad range of molecular properties of importance in several scientific areas. Examples sampled from our recent and past efforts in this area will be presented.