武汉物数所理论交叉学术交流系列报告

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A computational chemist´s guide to accurate thermochemistry for organic molecules

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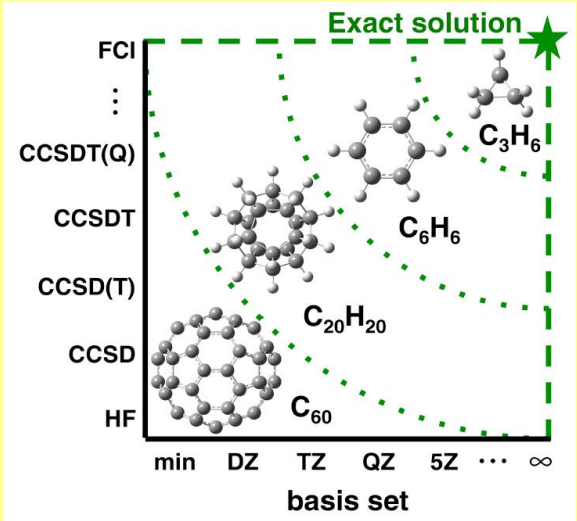
新波谱楼M-1017报告厅

About the speaker: Prof. Amir Karton currently holds an Australian Research Council Future Fellowship. He has published more than 100 articles in prestigious international journals. These articles have been cited over 3,100 times in the scientific literature and generate an H-index of 31. His research interests are focused on the development of quantum chemical theory for the calculation of highly accurate chemical properties and the application of these procedures to problems of chemical structure, mechanism, and design. These theories have been applied for solving challenging chemical problems that span several disciplines, ranging from biochemistry to nano-chemistry. Amir received a number of prestigious awards including the Le Fèvre Medal from the Australian Academy of Science (2018), the Vice-Chancellor's Early Career Investigators Award (UWA, 2016), and the Outstanding Young Investigator Award (UWA, 2013). For more information go to Amir's webpage: http://www.chemtheorist.com.

Abstract: **Composite ab initio methods are multistep theoretical procedures specifically designed to obtain highly accurate thermochemical and kinetic data with confident sub-kcal mol^{-1} or sub-kJ mol^{-1} accuracy. These procedures include all energetic terms that contribute to the molecular Binding energies at these levels of accuracy (e.g., CCSD(T), post-CCSD(T), core-valence, relativistic, spin-orbit, Born-Oppenheimer, and zero-point vibrational energy corrections). Basis-set extrapolations (and other basis-set acceleration techniques) are used for obtaining these terms at sufficiently high levels of accuracy. Major advances in computer hardware and theoretical methodologies over the past decade have enabled the application of these procedures to medium-sized organic systems (e.g., ranging from C_{60} to amino acids and DNA bases). With these advances, there has been a proliferation in the number of developed composite ab initio methods. In this talk I will give an overview of the accuracy and applicability of the various types of composite ab initio methods that were developed in recent years. General recommendations to guide selection of the most suitable method for a given problem will be presented, with a special emphasis on organic molecules [1].**



[1]. Karton, A. WIREs. Comput. Mol. Sci. 2016, 6, 292.

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