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NCCR MARVEL Distinguished Lecture

Interactive and Automated Exploration of Reaction Mechanisms

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Abstract: A prominent focus of molecular science has been the understanding and design of functional molecules and materials. This brings about new challenges for theoretical chemistry. As the electron correlation problem prevails, we are faced with the necessity to obtain theoretical results of predictable accuracy for molecules of increasing size and number. Moreover, the molecular composition, which is required as input for a quantum chemical calculation, might not be known, but the target of a design attempt. Then, the relevant chemical processes are not necessarily known, but need to be explored and identified. Whereas parts of these challenges have already been addressed by the development of specific methods (such as linear scaling or high-throughput screening), the fact that an enormous multitude of structures featuring various types of electron correlation needs to be considered calls for integrated approaches. This holds particularly true for predictions on complex chemical processes that encode function (e.g., through reaction networks). In my talk, I will discuss such challenges and present some of our latest developments that range from automated and interactive explorative approaches with error control for density functional theory to automated benchmarking based on black-box density matrix renormalization group calculations including dynamic correlation.