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Challenges in attochemistry and its theoretical description

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The absorption of light excites the electrons of a molecule. As a result, the distribution of electrons and thus the reactivity of the molecule in these electronically excited states differ significantly from the ones in the ground state. Thanks to this conceptually simple yet complex process, photochemistry has considerably broadened the spectrum of possible reactions, as compared to thermal chemistry. Yet, photochemical reactions are limited by the nature and finite number of electronic excited states in molecules. Because of the time-energy uncertainty principle, attosecond and subfemtosecond pulses have a large spectral width and therefore populate several electronic excited states in a simultaneous and coherent manner; this is called an "electronic wavepacket". By interference, the electronic distribution of a wavepacket is not the simple average of the individual electronic distributions of the different states: an electronic wavepacket is a new type of initial electronic state, with a new nature. What would be the reactivity of a molecule in this new electronic state? With the technological advances of attoscience, the concept of attochemical control, also called "charge-directed reactivity"has been demonstrated experimentally and theoretically mostly on diatomic. Although highly challenging, extending this to chemical reactions in polyatomic molecules is the ambitious goal of attochemistry. In this presentation, we will discuss the outstanding challenges in the field of attochemistry, and in particular its theoretical description.

Presenter: VACHER, Morgane (Nantes U)