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**Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations** MICHAEL OLIVEIRA, Department of Physics, University of Liege, Belgium, KSENIA KOMAROVA-VLADIMIROVA, FRANCOISE REMACLE, Department of Chemistry, University of Liege, Belgium, MATTHIEU VERTRAETE, Department of Physics, University of Liege, Belgium — The London-van der Waals dispersion forces arising from instantaneously induced dipoles in molecules are a key ingredient in a wide range of phenomena in physics, chemistry, and biology. Therefore, the ability to control and manipulate dispersion forces between atoms and molecules is of great importance. Because those dispersion interactions depend crucially on the electronic properties of the molecular systems, a simple route to achieve this would consist in manipulating their electronic states. The recent development of ultra-short optical pulses has given researchers unprecedented control over the electronic degrees of freedom. These pulses, tailored in their frequency and envelope, allow the generation of a strongly out of equilibrium population of electronic states. In this talk we show how the Hamacker constants characterizing the London-van der Waals interaction between two molecules subject to an optical pulse can be calculated using time-dependent density functional theory (TD-DFT) or standard quantum chemistry methods and present several test cases of molecules subjected to IR and UV attosecond pulses.

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