

# Electronic coherences built by an attopulse shape the entanglement between electronic and nuclear degrees of freedom and the force on the nuclei

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Short attosecond (as) or few femtoseconds (fs) IR and UV pulses have a broad energy bandwidth which allows exciting a superposition of several electronic states in neutral molecules and molecular cations.[1] The nature of the states excited can be controlled by tuning the pulse parameters. This opens the way to novel avenues for control by engineering of electronic coherences between selected electronic states to steer charge migration on a purely electronic time scale.[2] As the nuclei begin to move, the electronic and nuclear motions are entangled and the engineered electronic coherences can be usefully exploited for directing the vibronic density through the network of non adiabatic interactions to specific products.

In order to design control schemes built on a selective photoexcitation of electronic coherences, we analyze the time evolution of the entanglement between nuclear and electronic degrees of freedom using singular valued decomposition (SVD) of the wave function[3] and the relative importance of the terms of the force exerted by the vibronic wave packet on the nuclei during and also after the pulse. I will discuss several examples of the role of initial entanglement induced by the interaction with an attopulse and the resulting force in the nuclei in the selective fragmentation of diatomic molecules,[4] the bond formation in a 4C ring closure induced by tuning the parameters of a few cycle deep UV pulse[5] and the ultrafast Jahn-Teller rearrangement of the methane cation.[6]

## References

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