# $H_2$ photoionization induced by XUV pulses and X-ray free electron lasers

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**Synopsis** We present a theoretical study on $H_2$ photionization taking into account coupled electron-nuclear motion and non-dipole effects. In the first part we study the effects of harmonic filtering in a pump-probe scheme using attosecond train pulses (ATP) in dipole approximation. In the second part we investigate nondipole effects in XUV and soft X-ray regimes.

The development of intense XUV sources through free electron lasers (FEL) and high-order harmonic generation (HHG) in the femtosecond (fs) and sub fs domains provides a unique tool to investigate non-linear laser matter interaction at ultra short time durations. Attosecond pulses provide the possibility for coherently and simultaneously control both electronic and nuclear dynamics, specifically populating different vibronic (electronic+vibrational) states [1], this makes mandatory the use of theoretical approaches beyond the Born-Oppenheimer approximation to be understood. On the other hand it is well-known that, in the XUV and soft X-rays domains, the dipole approximation must be carefully used. In particular, nondipole effects in atom and molecules result in asymmetries of the photoelectron distributions (see [2] for the cases of He or $H_2$, and references therein).

In this work, we present ab initio calculations performed on $H_2$ [3] to investigate the possibility of control excitation and ionization yields in two different cases. In the first case we investigated the effect of filtering different harmonics in a pump-probe scheme using VUV ATP. The higher state selectivity of ATP compared to single broad-bandwidth attosecond pulses together with the capabilities of IR sources to trace and drive the coupled electron and nuclear motion initiated by a VUV ATP makes this technique perfect to control excitation and ionization yields on attosecond timescales by means of electron wave packets interference [1]. For the second case we follow our recent research on stimulated Compton scattering in hydrogen [4] where we have shown that the diamagnetic term $\mathbf{A}^2$ (where $\mathbf{A}$ the vector potential of the field), usually neglected in dipole approximation, plays a crucial role in this context. These studies are now extended to the molecule $H_2$, results will be presented and discussed at the conference.

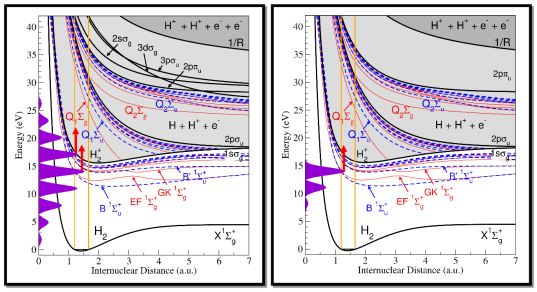


**Figure 1**. Schematics of the pump-probe simulation. Upper panels represent the temporal profile of the pump and probe laser fields. Lower panels represent the spectrum of said pulses superimposed to the energy diagram of $H_2$. Right figures correspond to the filtered case and left figures correspond to the unfiltered case.

## References

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