

# Theoretical Physics Seminar

## **Correlation effects in strong field enhanced ionization of molecules : A time-dependent generalized-active-space configuration-interaction study.**

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**When:** 12 October 2017, 4:00 pm

**Place:** Room No. 469

In this talk, I will present recent results on the correlation effects in strong field ionization of diatomic molecules. In this work, we have studied  $\mathrm{H}_2$ ,  $\mathrm{LiH}$ , and  $\mathrm{HF}$  molecules, aligned collinearly with the linear polarization of the external field. To elucidate the possible role of electron correlation in the enhanced-ionization (EI) phenomena we consider different levels of approximation with the time-dependent generalized-active-space configuration-interaction (TD-GASCI) method. The results of our studies show that correlation is important and they also demonstrate significant deviations between the results of the single-active-electron approximation and more accurate configuration-interaction methods. We will further investigate the role of low-lying excited states in the EI phenomena. With the inclusion of correlation we show strong carrier-envelope-phase effects in the EI of the asymmetric heteronuclear  $\mathrm{LiH}$  molecule. The correlated calculation shows an intriguing feature of cross-over in enhanced ionization with two carrier-envelope-phases at critical inter-nuclear separation.

**All are welcome**