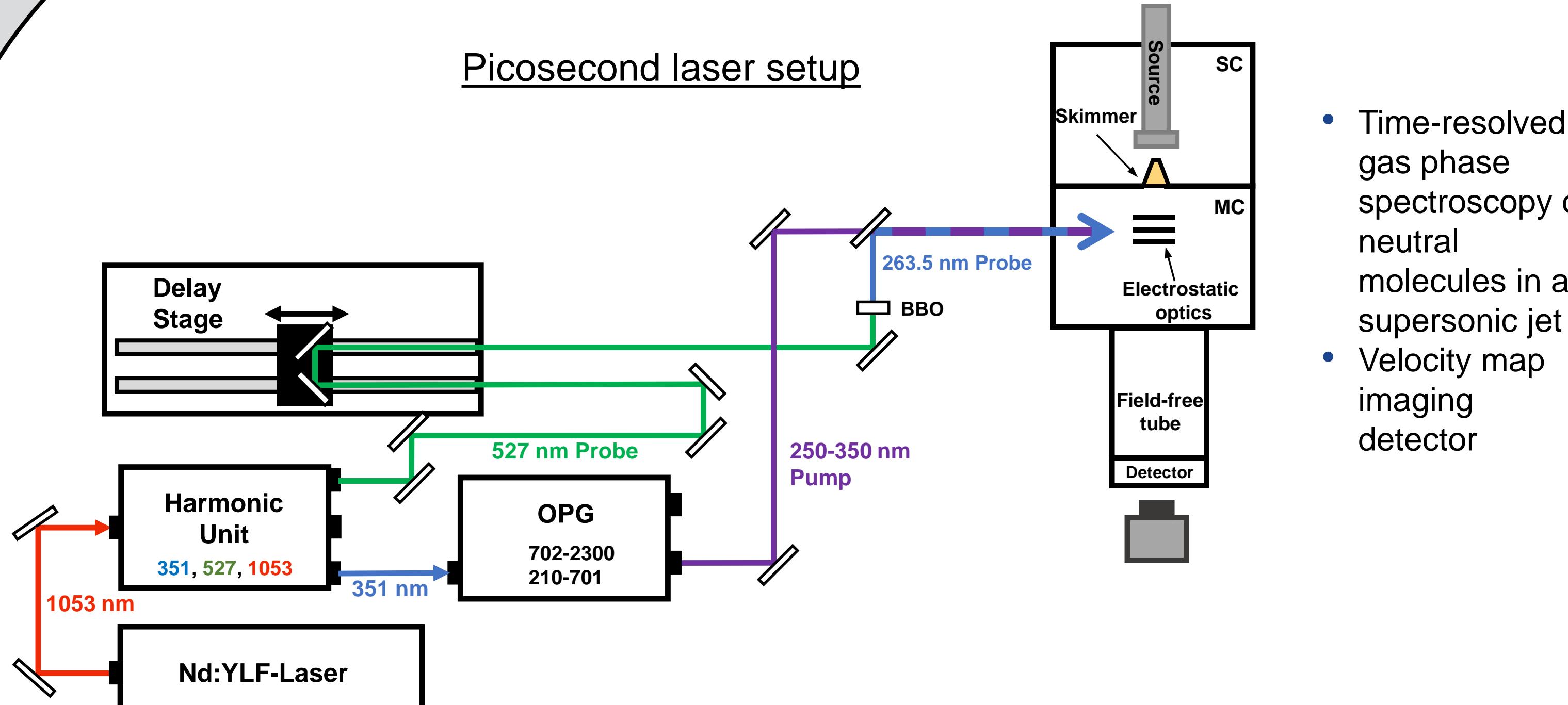


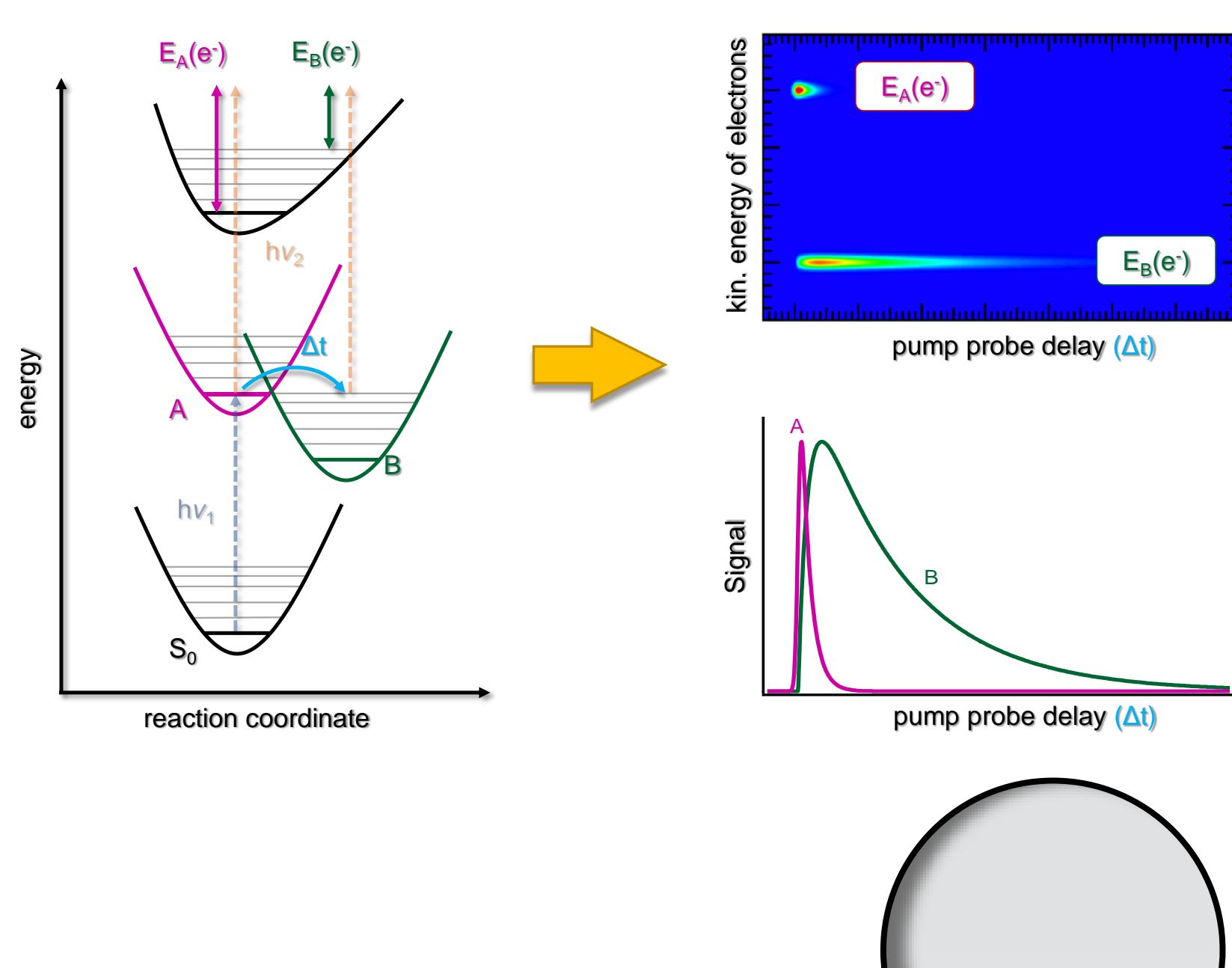
# Excited state dynamics of BN-9,10-naphthalene: The impact of replacing CC by BN

F. Sturm, M. Bühler, C. Stapper, J. Schneider, H. Helten, M. Röhr, I. Fischer  
Institute for Physical and Theoretical Chemistry, Julius-Maximilians-Universität Würzburg, 2023

## Experimental Methods

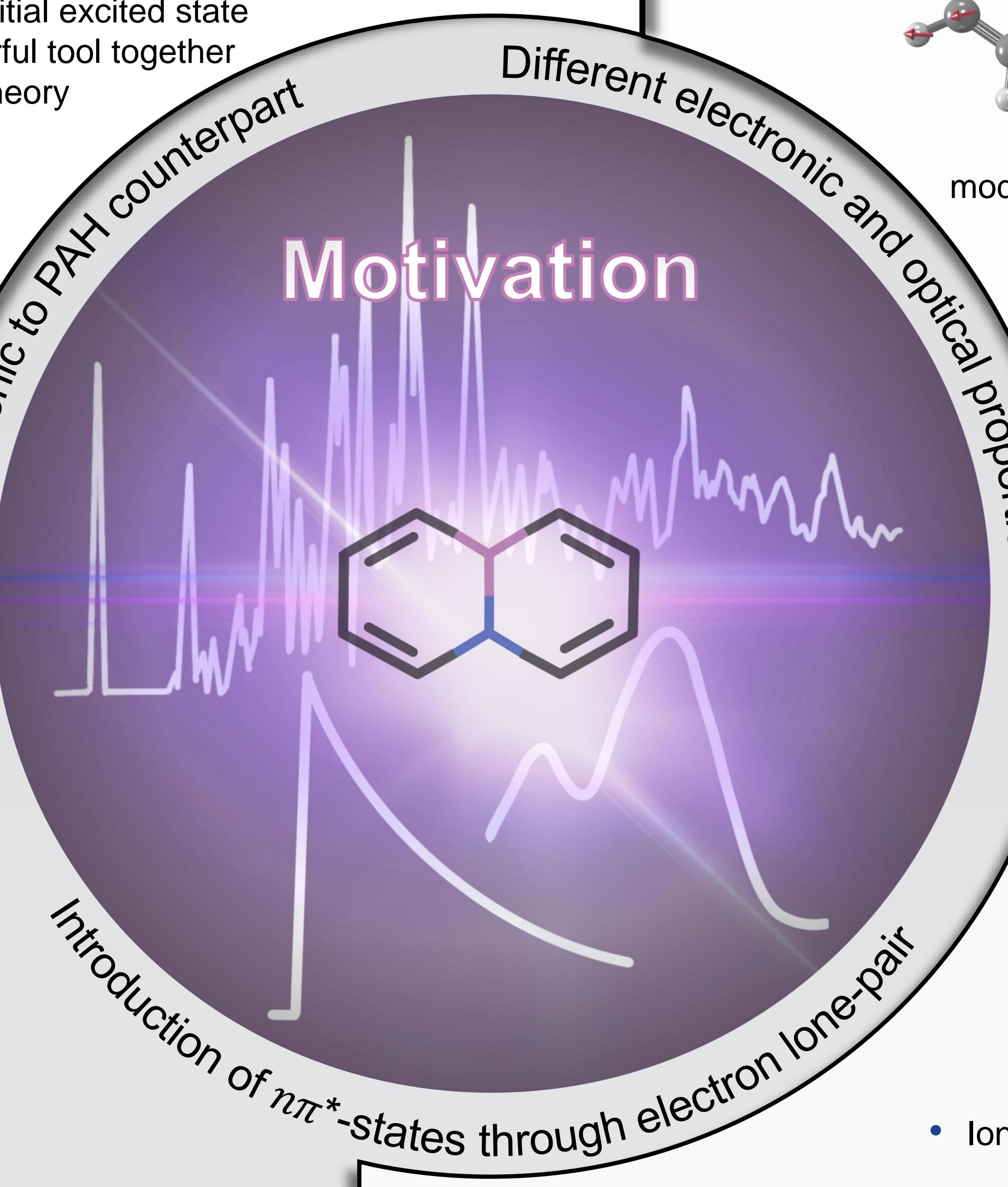
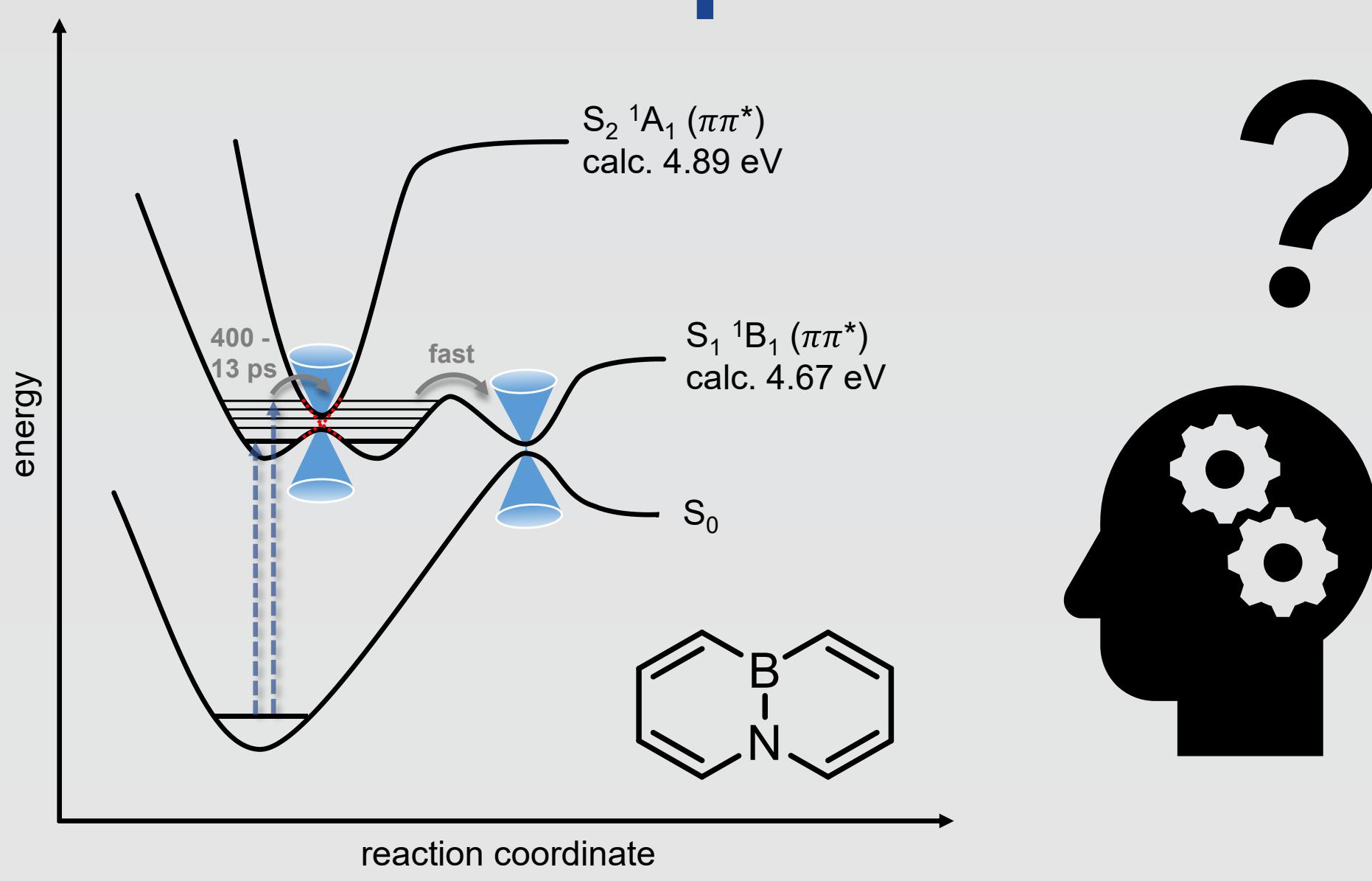


### Time-resolved VMI (velocity map imaging)

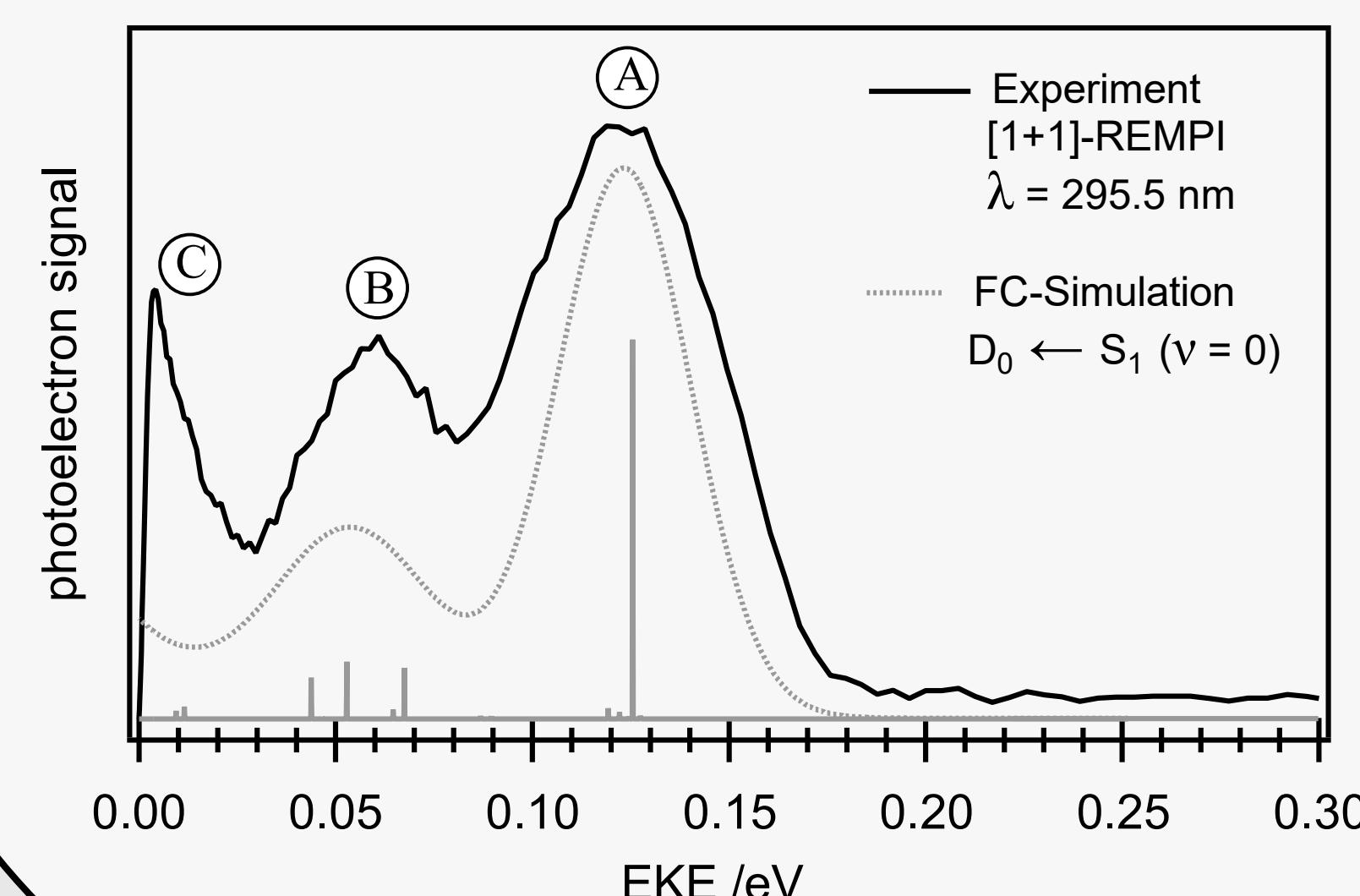


- Information of time-constants and initial excited state
- Powerful tool together with theory

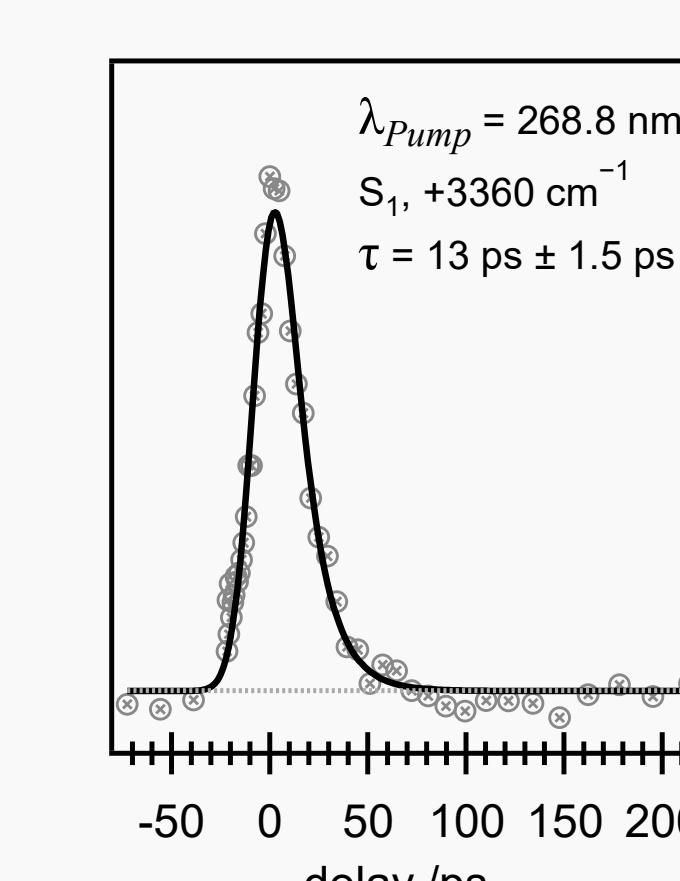
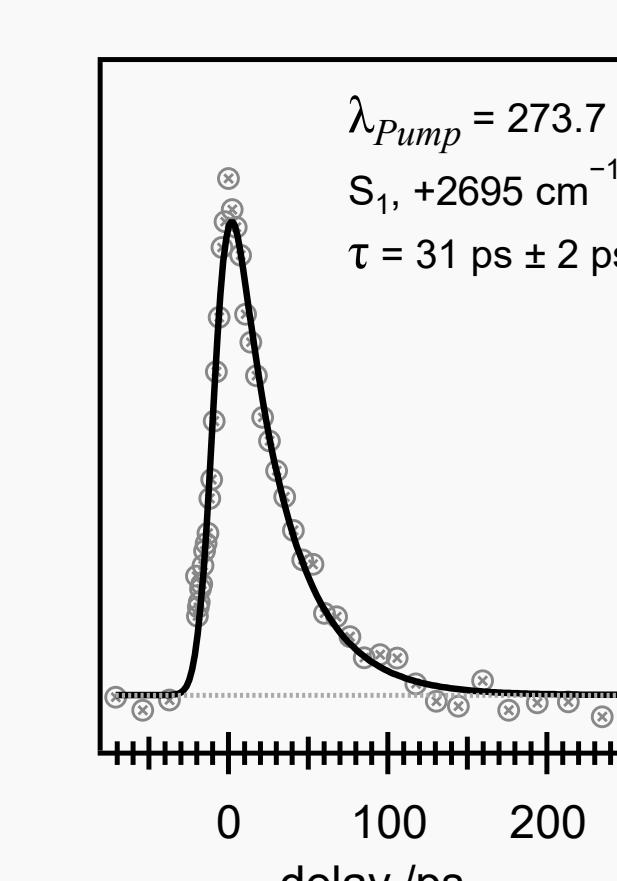
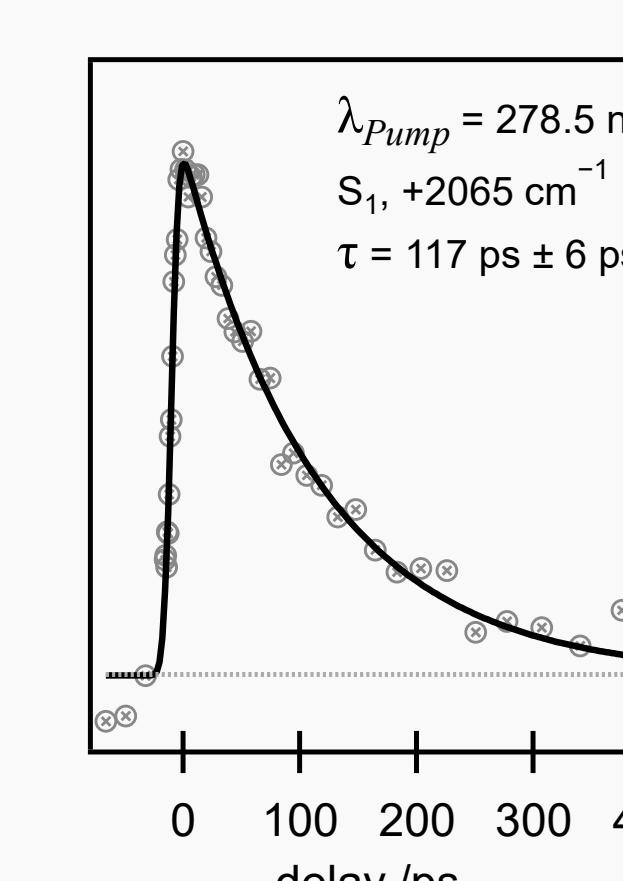
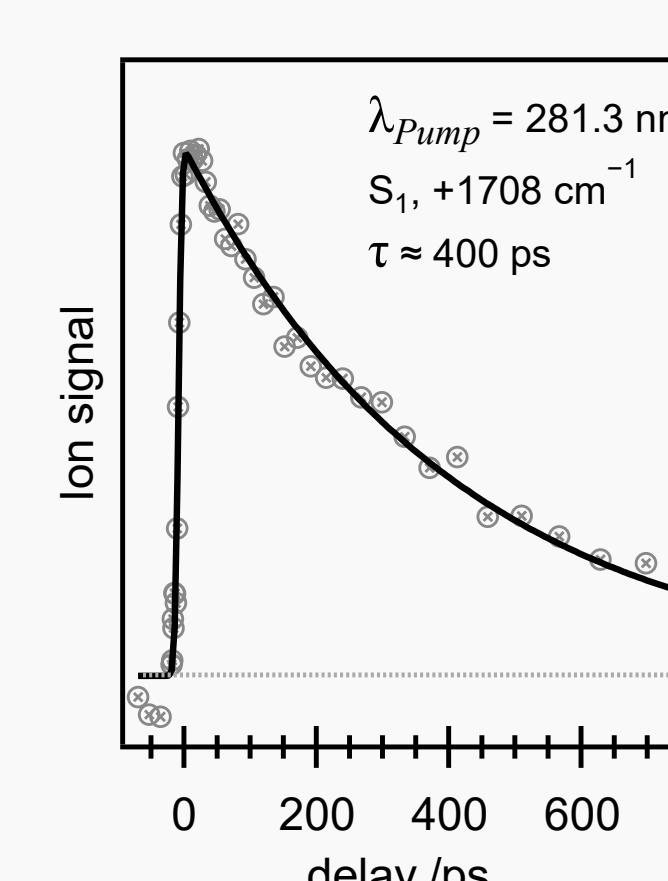
## Interpretation



## Photoelectron spectrum

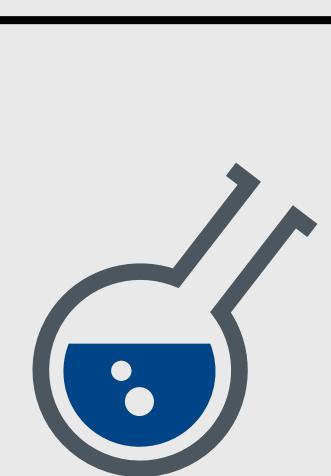
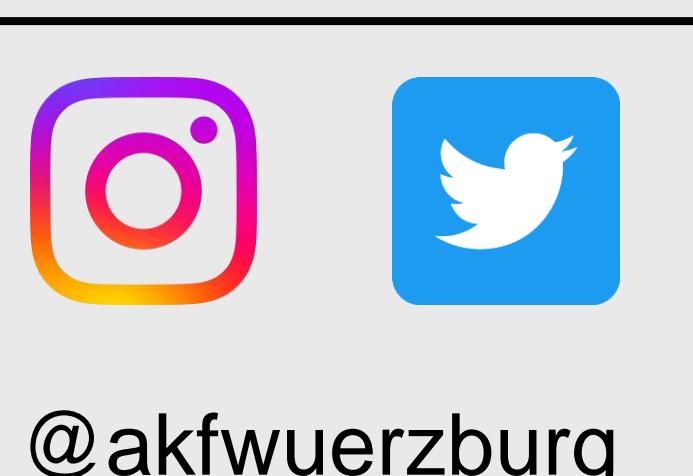


- Experimental ionization:  $IE_{ad} = 8.27 \pm 0.025$  eV
- Franck-Condon simulation: TD-DFT on the wB97XD and aug-cc-pVTZ level of theory



- Dynamics depend strongly on excitation energy → with higher excitation energy all time constants decrease monoexponentially to zero
- First time constant is observable at 1708 cm⁻¹ (0.21 eV) above S1 origin

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## Affiliation



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