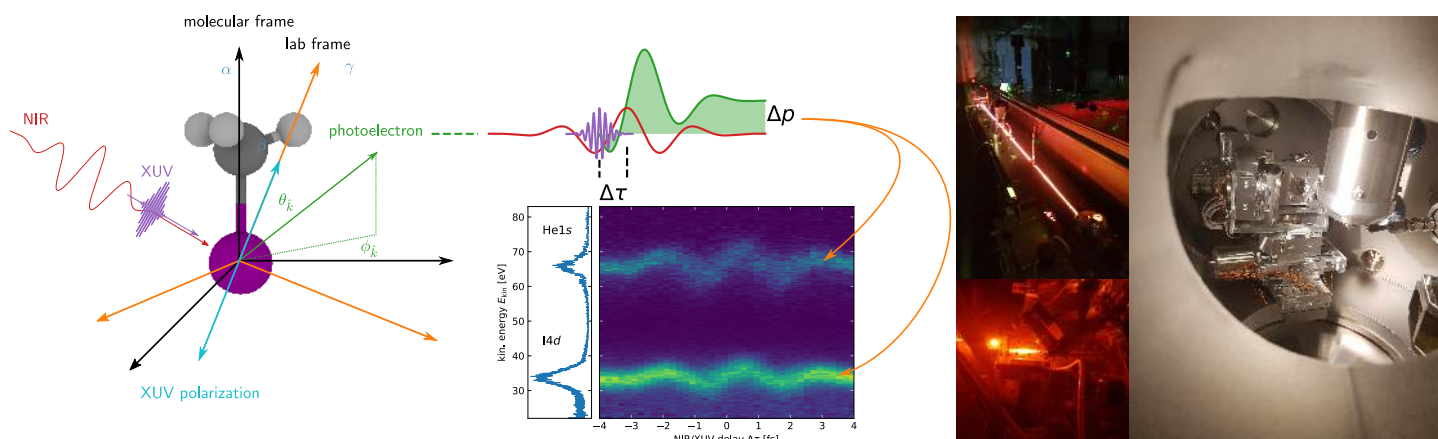


Master's thesis

Absolute photoemission timing on Iodomethane and Iodoethane

Chair for laser- and x-ray physics, E11



Description

This thesis concerns itself with the experimental assessment of the absolute timing of the I4d photoemission from Iodomethane and Iodoethane for photon energies between 90 eV and 120 eV. It is part of a larger effort to understand the dynamics of photoemission from small molecules and offers the opportunity to study not only the influence of the molecular environment on the observable photoemission delay, but also the so-called *giant resonance* (c.f. e.g. [1]) in the I4d \rightarrow εf photoemission in the time domain – a phenomenon of great interest in atomic physics.

The excitation-energy dependent photoemission delay, which is on the order of attoseconds ($1 \text{ as} = 1 \times 10^{-18} \text{ s}$), can only be accessed in an experiment using sophisticated tools from the field of ultrafast physics: our setup implements the attosecond streak camera principle (c.f. [4, 8]) and an absolute referencing scheme established recently [6]. It is one of the few in the world where such experiments can be conducted.

The experimental work will be complemented by state-of-the-art numerical studies of the photoemission process in these molecules in order to complete the picture, where state-of-the-art methods will be applied for the determination of molecular electronic structure [3, 7] and the treatment of the photoionization process [5, 2].

Keywords

Experiment pulsed lasers, attosecond physics, nonlinear optics, photoelectron spectroscopy, *giant resonances*

Numerics/Data evaluation Hartree-Fock, GAMESS, ePolyScat, python

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References

- [1] Jean Patrick Connerade, Jean-Marc Esteve, and RC Karnatak. *Giant resonances in atoms, molecules, and solids*. Vol. 151. Springer, 2013.
- [2] F. A. Gianturco, R. R. Lucchese, and N. Sanna. "Calculation of low-energy elastic cross sections for electron-CF4 scattering". In: *The Journal of Chemical Physics* 100.9 (1994), pp. 6464–6471. DOI: 10.1063/1.467237.
- [3] Mark S. Gordon and Michael W. Schmidt. "Chapter 41 - Advances in electronic structure theory: GAMESS a decade later". In: *Theory and Applications of Computational Chemistry*. Ed. by Clifford E. Dykstra et al. Amsterdam: Elsevier, 2005, pp. 1167–1189. ISBN: 978-0-444-51719-7. DOI: <https://doi.org/10.1016/B978-044451719-7/50084-6>.
- [4] E. Goulielmakis et al. "Direct Measurement of Light Waves". In: *Science* 305.5688 (2004), pp. 1267–1269. ISSN: 0036-8075. DOI: 10.1126/science.1100866.
- [5] Alexandra P. P. Natalense and Robert R. Lucchese. "Cross section and asymmetry parameter calculation for sulfur 1s photoionization of SF6". In: *The Journal of Chemical Physics* 111.12 (1999), pp. 5344–5348. DOI: 10.1063/1.479794.
- [6] M. Ossiander et al. "Attosecond correlation dynamics". In: *Nature Physics* 13.3 (Mar. 2017), pp. 280–285. ISSN: 1745-2481.
- [7] Michael W. Schmidt et al. "General atomic and molecular electronic structure system". In: *Journal of Computational Chemistry* 14.11 (1993), pp. 1347–1363. DOI: 10.1002/jcc.540141112.
- [8] M. Schultze et al. "Delay in Photoemission". In: *Science* 328.5986 (2010), pp. 1658–1662. ISSN: 0036-8075. DOI: 10.1126/science.1189401.