

**SLS Symposium on**  
**In-situ and dynamics**  
**with soft X-ray spectroscopy**

**Tuesday, October 10<sup>th</sup>, 2017**

**10:00 to 11:45, WBGB/019**

**10:00 Towards Biased-ARPES for Silicon Carbide Device Analysis**

*Judith Woerle, M. Caputo, A. Tsibizov, S. Nida, F. Bisti, M.-A. Husanu, V. N. Strokov, H. Sigg, J. Gobrecht, U. Grossner and M. Camarda*

**10:30 In situ investigation of supersaturated calcium carbonate solutions by X-ray absorption spectroscopy**

*Katja Henzler, E. O. Fetisov, M. Galib, M. D. Baer, C. Borca, J. M. Xto, B. A. Legg, S. Pin, J. L. Fulton, G. K. Schenter, N. Govind, J. I. Siepmann, C. J. Mundy, T. Huthwelker, J. J. De Yoreo*

**11:00 Coffee**

**11:15 Electronic states of the xylyl radicals and cations**

*Mathias Steglich, P. Hemberger*

# Towards Biased-ARPES for Silicon Carbide Device Analysis

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Although Silicon Carbide (SiC) represents the most mature material for wide-bandgap high-voltage power electronic devices, the inversion channel of SiC metal-oxide-semiconductor field effect transistors (MOSFETs) is still strongly affected by low mobility and low performance reliability [1]. These problems are related to the large amount of both interface defects and near-interface traps generated during thermal oxidation whose origin is still under debate [2].

Soft X-Ray angle-resolved photoemission spectroscopy (SX-ARPES), with its unique capability to directly resolve the energy-momentum space and image the electronic structure of materials, has been demonstrated to be a useful tool to study the nature of interface defects at the SiO<sub>2</sub>/SiC interface, showing no signs of ST-derived surface states (see Fig. 1 and [3]). A very promising extension to this technique is biased-ARPES where the band structure of the material is investigated under electrical biases resulting in higher occupation densities and a shift of the Fermi energy level above the conduction band.

Here we present our current experimental efforts towards an in-situ analysis of a SiC MOSFET with SX-ARPES which are carried out at the ADRESS beamline at the Swiss Light Source [4] demonstrating the feasibility of this novel defect mapping technique. In addition, theoretical considerations on the impact of X-ray illumination on carrier densities and band bending in the semiconductor device are discussed.

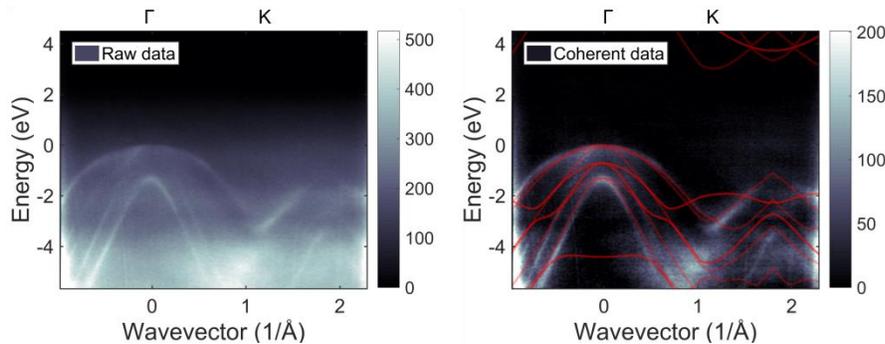


Figure 1: Experimental valence band spectra of the SiO<sub>2</sub>/SiC(0001) interface along  $\Gamma$ -K for  $d = 2$  nm and  $h\nu = 470$  eV. (left) Raw ARPES intensity. (right) Coherent fraction of the ARPES image with the superimposed theoretical band structure of 4H-SiC. No signs of additional  $k$ -dispersive structures neither in the bandgap of SiC nor in its valence band region was detected.

[1] G. Liu, B.R. Tuttle and S. Dhar, *Appl. Phys. Rev.* **2**, 021307 (2015)

[2] T. Kimoto and J. A. Cooper, *Fundamentals of Silicon Carbide Technology* (Wiley, 2014)

[3] J. Woerle, F. Bisti, M. A. Husanu, V. N. Strocov, C. W. Schneider, H. Sigg, J. Gobrecht, U. Grossner, and M. Camarda, *Applied Physics Letters* **110**, 132101 (2017)

[4] V. N. Strocov, M. Kobayashi, X. Wang, L. L. Lev, J. Krempasky, V. V. Rogalev, T. Schmitt, C. Cancellieri, and M. L. Reinle-Schmitt, *Synchrotron Radiation News* **27**, 31 (2014).

## In situ investigation of supersaturated calcium carbonate solutions by X-ray absorption spectroscopy

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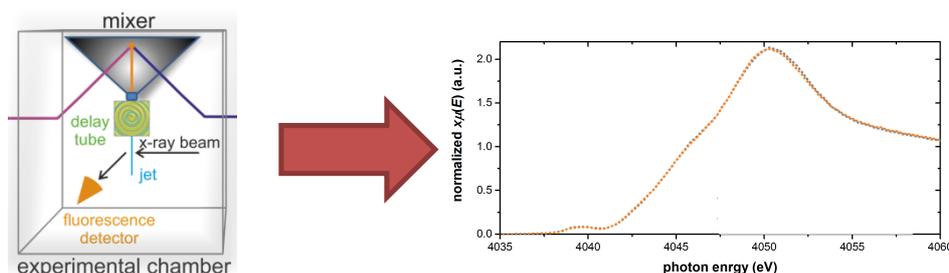
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The mechanism of calcium carbonate nucleation from aqueous solutions has recently been proposed as a multi-stage pathway invoking clusters as intermediate species [1]. However, until now any clusters, which are believed to form just after the nucleation event, evaded direct experimental observation by means of both scattering and spectroscopic techniques. Hence, there are no direct experimental investigations which reveal the structural arrangement of the ions in these clusters, which comprise the very first moment of crystallization. Candidate structures include simple ion pairs, as predicted by classical models [2], but also more complex potentially polymer like structures, as proposed in the recent literature [3] Here we provide an in-situ experimental study of the structure of supersaturated CaCO<sub>3</sub> solution by X-ray absorption spectroscopy. Based on the experimental finding we present conclusions about the structure of carbonate complexes in supersaturated solution and compare the experimental results with theoretical models.



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[2] L. N. Plummer, E. Busenberg, *Geochim. Cosmochim. Acta* 46, 1011-1040 (1982).

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# Electronic states of the xylyl radicals and cations

Mathias Steglich, Patrick Hemberger

Paul Scherrer Institute, VUV Beamline

## Abstract

Xylenes are used as fuel additives because of their high octane ratings and to improve antiknock performances of combustion engines. The first step in their pyrolysis is the formation of the resonantly stabilized xylyl radicals shown in Fig. 1, which are key species that determine the following combustion processes, especially the formation and emission of harmful PAHs. A few experimental studies dealt already with the decomposition dynamics of these radicals on a  $\mu\text{s}$  scale [e.g., 1]. However, it is also of fundamental interest to understand the ultrafast processes that characterize the first steps of unimolecular reactions in the pyrolysis of these long-lived combustion intermediates. To this end, femtosecond laser pulses are usually applied in pump-probe experiments [2, 3]. Conducting such experiments requires knowledge about the electronic states involved. In general, electronic spectroscopy of benzylic radicals and ions can serve as reference and provide valuable input for theoretical quantum chemistry. In this talk, I will present the electronic spectra of the xylyl radicals up to 5 eV, obtained by resonant one-color two-photon ionization (R2PI). Electronic states of the corresponding cations have been probed by threshold photoelectron (TPE) spectroscopy up to 4 eV above the singlet ground states. Supported by quantum chemical calculation, these results shed light onto the excited state potential energy surfaces and reveal interesting differences between the three isomers. The findings support femtosecond time-resolved studies, which are currently carried out in our laser laboratory and which I will also discuss briefly.

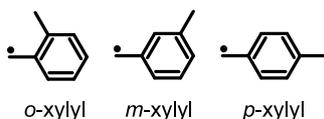


Figure 1: Molecular structures of the resonantly stabilized xylyl radicals.

## References

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