

In situ monitoring of electrochemically generated carbene by XPS

Pinar Aydogan Gokturk^{1*}, Selin Ezgi Donmez¹, Yunus Emre Turkmen¹, Burak Ulgut¹, Sefik Suzer¹.

¹ Department of Chemistry, Bilkent University, 06800 Ankara, Turkey

*e-mail: pinar.aydogan@bilkent.edu.tr

Ionic liquids provide a platform for fundamental electrochemical studies in vacuum. In this present work, we report an in-situ X-ray photoelectron spectroscopic (XPS) investigation of N-heterocyclic carbene(NHC) generation from the electrochemical reduction of imidazolium based ionic liquids (ILs) through changes in oxidation state of nitrogen atoms. The IL serves as an electroactive material as well as the electrolyte in the cell between a Si substrate which is connected to the instrument ground and a gold wire connected to the sample holder for electrical connection. Through the course of the electrochemical reaction, the positive charge on imidazolium cation is neutralized to give free NHC as reflected by the distinct shifts in the N 1s and C 1s binding energies. The observations are further supported by colorful adduct formation of carbenes with CS₂, reversible redox peaks in the voltammogram and the density functional theory calculations. The presented structure and XPS measurements can lead on understanding of the mechanism for various electrochemical reactions.

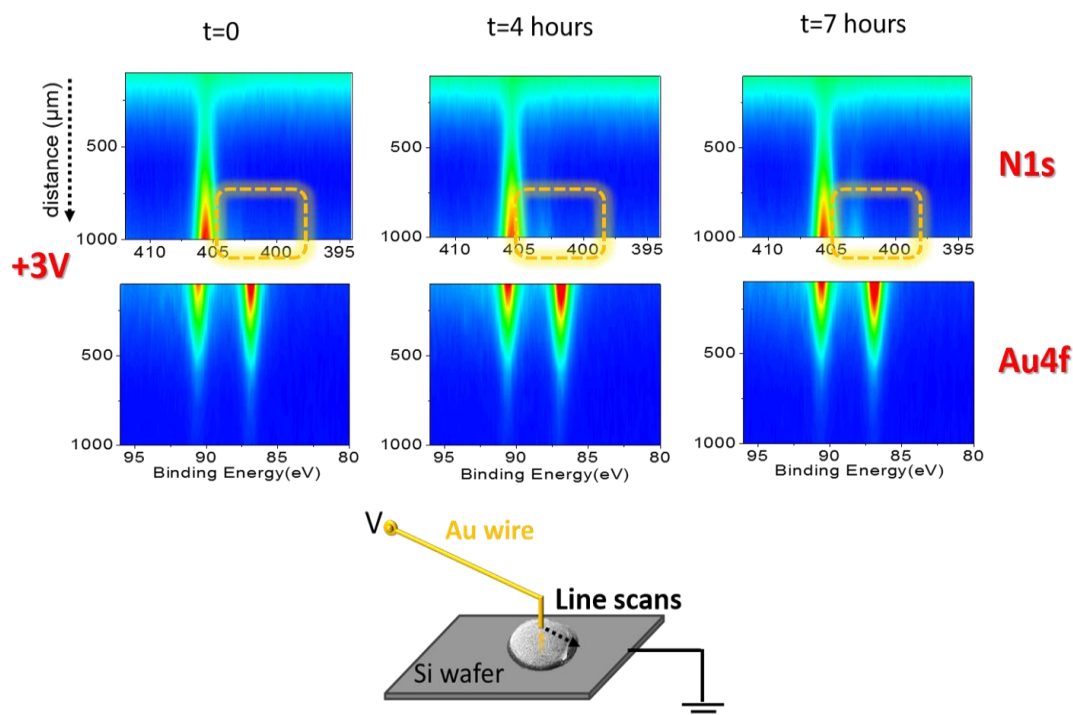


Figure 1 XP Spectra of the N1s and Au4f regions along the line designated under +3 V in different times

Acknowledgements

This work is partially supported by TUBITAK (The Scientific and Technological Research Council of Turkey) via the Grant No: 215Z534