

# Dissociative adsorption of CO<sub>2</sub>: The role of the steps

Benjamin Hagman<sup>1</sup>, Alvaro Posada-Borbón<sup>2</sup>, Andreas Schaefer<sup>3</sup>, Natalia M. Martin<sup>3</sup>,  
Henrik Grönbeck<sup>2</sup>, Edvin Lundgren<sup>1</sup>, Johan Gustafson<sup>1</sup>

<sup>1</sup>*Synchrotron Radiation Research, Lund University, SE-221 00 Lund, Sweden*

<sup>2</sup>*Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology,  
SE-412 96 Gothenburg, Sweden*

<sup>3</sup>*Department of Chemistry and Chemical Engineering and Competence Centre for Catalysis,  
Chalmers University of Technology, SE-412 96 Gothenburg, Sweden*  
benjamin.hagman@sljus.lu.se

Due to the urgent problem of global warming, a demand of reducing the release of the greenhouse gas CO<sub>2</sub> into the atmosphere has emerged. A potential approach to limit the CO<sub>2</sub> release is to convert it into useful chemical products, such as methanol, instead of releasing it into the atmosphere. However, the recycling of CO<sub>2</sub> is a challenging task as the molecule is rather inert, which makes it difficult to activate for reduction and subsequent hydrogenation. The most used metal for this activation is Cu, and, hence, a fundamental understanding of how CO<sub>2</sub> interacts with Cu surfaces would promote the development of new catalysts for the reduction of CO<sub>2</sub> [1].

We have previously studied the CO<sub>2</sub> interaction with a Cu(100) surface using Ambient Pressure X-ray Photoelectron Spectroscopy [2], and the analysis, supported by Density Functional Theory (DFT) calculations [3], strongly indicates that the steps on the surface are responsible for the CO<sub>2</sub> adsorption and the subsequent dissociation.

In the present contribution we confirm experimentally the importance of steps using APXPS, exposing a stepped Cu(911) surface to CO<sub>2</sub> at elevated pressures. We observe that CO<sub>2</sub> chemisorbs as the activated species CO<sub>2</sub><sup>-δ</sup> on the surface, and dissociates forming adsorbed atomic oxygen and CO that desorbs. We demonstrate that the CO<sub>2</sub> adsorption is significantly facilitated by the presence of the steps on the Cu(911) surface as compared to the flat Cu(100). The effect of the facilitated CO<sub>2</sub> adsorption on the subsequent dissociation will be discussed.

## References:

- [1] Marc D. Porosoff, Binhang Yang, Jingguang G. Energy Environ. Sci. **9**, 62 (2016).
- [2] Benjamin Hagman, et al, in manuscript.
- [3] Alvaro Posada-Borbón, et al, in manuscript.