

# Exploring the Electron Spin Polarization in Chiral Oxide Layers Employed as Spin-Selective Catalysts

P. V. Möllers<sup>\*1</sup>, J. Wei<sup>2</sup>, S. Ghosh<sup>2</sup>, S. Salamon<sup>3</sup>,  
M. Bartsch<sup>1</sup>, H. Wende<sup>3</sup>, D. H. Waldeck<sup>2</sup>, H. Zacharias<sup>1</sup>

<sup>1</sup> Center for Soft Nanoscience (SoN), Universität Münster, 48149 Münster, Germany

<sup>2</sup> Chemistry Department, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, United States

<sup>3</sup> Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE),  
Universität Duisburg-Essen, Duisburg, Germany

\*paul.moellers@uni-muenster.de

The chirality-induced spin selectivity (CISS) effect reveals a relation between the electron spin and the frame of reference of single chiral molecules and solid-state materials. It introduces new means for controlling the outcome and efficiency of spin-dependent chemical reactions, e.g., photoinduced water splitting.

First demonstration experiments for an improved water splitting, employing either chiral cupric oxide (CuO) or chiral cobalt oxide (CoO<sub>x</sub>) layers [1,2], have proven the feasibility of this approach. However, a thorough understanding of the origin of the spin polarization generated in these oxide layers is still lacking.

In this talk, the concept of spin-selective electrocatalysis is briefly introduced. We present photoemission measurements which demonstrate that spin-polarized currents can be obtained from chiral CuO [1,3] and CoO<sub>x</sub> [2] layers and explore the underlying mechanisms.

For CuO thin films, correlating the SP values with electron energy spectra reveals that the measured spin polarization values could be rationalized assuming an intrinsic spin polarization in the chiral oxide layer and a chirality-induced spin selectivity (CISS)-related spin filtering of the electrons. We hypothesize that the intrinsic contribution to the spin polarization reflects a magnetic order which is absent within achiral but otherwise identical layers [3]. In chiral CoO<sub>x</sub> layers, the spin polarization was found to depend on the cobalt oxidation state, which allows for reversible switching of the preferred spin orientation. The results support efforts towards a rational design of further spin-selective catalytic oxide materials.

[1] K. B. Ghosh et al., J. Phys. Chem. C **123**, 3024–3031 (2019)

[2] S. Ghosh et al., J. Phys. Chem. C **124**, 22610–22618 (2020)

[3] P. V. Möllers et al., ACS Nano **16**, 12145–12155 (2022)

[4] P. V. Möllers et al., Isr. J. Chem. **62**, e202200062 (2022)