Infrared Spectroscopy and Quantum Chemical Calculations of CO and HCOOH Adsorption on Cerium Oxide Surfaces

Z. Yu[1], J. Vázquez Quesada[2], X. Kraft[2], S. Gojare[2], S. Chen[1], W. Li[1], A. Nefedov[1], C. Wöll[1], K. Fink[2], Y. Wang[1]

[1]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

[2]Institute of Nanotechnology (INT), Karlsruher Institut für Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany
E-Mail: yuemin.wang@kit.edu

A fundamental understanding of the surface structure and active sites of ceria-based catalysts is one of the most significant and challenging subjects in heterogeneous catalysis. Given the great complexity of ceria nanomaterials, a thorough surface science study based on well-controlled model systems is required to provide reliable and comprehensive reference data [1-6]. Here, we present systematic polarization-resolved IRRAS (infrared reflection absorption spectroscopy) investigations of CO and HCOOH adsorption on various low-index ceria single crystal surfaces. Interpretation of the experimental data was aided by quantum chemical calculations in the framework of an embedded cluster approach. Building upon the accurate reference data acquired for various model systems, we aim to gain profound insights into the interaction of CO and HCOOH with ceria nanoparticles measured by in situ IR transmission (UHV-FTIRS) and high-pressure DRIFTS. The understanding of CO interactions with cerium oxide surfaces is advanced by bridging the so-called materials and pressure gaps [5]. The different CO vibrational bands were used to monitor surface structural changes occurring at elevated pressures and temperatures. The formation of formate species in diverse adsorption configurations will be discussed in detail.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 426888090 – SFB 1441.

[1] Y. Wang, C. Wöll, Chem. Soc. Rev. 2017, **46**, 1875-1932. DOI: 10.1039/C6CS00914J.
[2] C. Wöll, ACS Catal. 2019, **10**, 168-176. DOI: 10.1021/acscatal.9b04016.
[3] C. Yang, N. López, W. Shen, C. Wöll, Y. Wang, *et al.*, J. Phys. Chem. Lett. 2020, **11**, 7925-7931. DOI: 10.1021/acs.jpclett.0c02409.
[4] P. G. Lustemberg, C. Yang, Y. Wang, C. Wöll, M. V. Ganduglia-Pirovano, J. Chem. Phys. 2023, **159**, 034704. DOI: 10.1063/5.0153745.
[5] L. Caulfield, E. Sauter, H. Idriss, Y. Wang, and C. Wöll, J. Phys. Chem. C 2023, **127**, 14023-14029. DOI: 10.1021/acs.jpcc.3c03567.
[6] J. Vázquez Quesada, S. Bernart, F. Studt, Y. Wang, K. Fink, to be submitted.