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ABSTRACT:

Quantification of Point Defects and their Dynamics in Mixed Conducting Oxides with X-Ray Spectroscopies

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Since in situ and operando variants of X-Ray spectroscopies have become more and more available, detection of ionic and electronic charge carriers in mixed conducting, nonstoichiometric oxides and their evolution during electrochemical processes have become a routine application.[1] The quantitative connection to defect chemistry as derived from classical electrochemical experiments, however, is not always straightforward[2], sometimes leading to ostensible discrepancies[3], mostly originating from hybridization and covalency effects, which are also dynamic.
Taking these effect into account, we will use late 3d transition metal oxide perovskites to showcase how a quantitative defect model of the near surface region can be derived from X-Ray absorption and photoemission spectroscopy (XAS and XPS, respectively). Proper identification and quantification of the charge carriers then allows us to conduct dynamic XPS experiments with millisecond resolution to track the oxygen surface exchange on well defined late 3d transition metal perovskites.

[1] D. N. Mueller, in Applications of X-ray Photoelectron Spectroscopy to Catalytic Studies, Catalytic Science Series Vol. 21, p. 457, S. Zafeiratos, Ed. (World Scientific, Singapore, 2023).
[2] J. Wang, D. N. Mueller, E. Crumlin, J. Eur. Ceram. Soc. 44, 116709 (2024).
[3] R. A. De Souza, D. N. Mueller, Nat. Mater. 20, 443–446 (2020).