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Operando XAS studies of direct synthesis of H2O2 over Pd catalysts

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Hydrogen peroxide (H₂O₂) is a widely used powerful, environmentally benign oxidizing agent. The liquid phase catalyzed direct synthesis of H₂O₂ from molecular hydrogen and oxygen constitutes an attractive greener alternative to the industrial anthraquinone autooxidation process. However, insufficient mechanistic details hinder the development of enhanced catalysts and the choice of suitable reaction conditions for the direct synthesis of H₂O₂. Furthermore, safety concerns related to formation of explosive H₂/O₂ mixtures severely restrict *in situ* / *operando* studies of the direct synthesis of H₂O₂ as well as its commercial application. In order to gain insight in the catalytic processes occurring during the H₂O₂ synthesis at the molecular level, we performed operando XAS studies of Pd catalysts in a continuous flow reactor at pressures of 10-40 bar. Water and ethanol were used as solvents. In both cases H₂:O₂ ratio was varied while the complementary on-line product analysis allowed deriving structure-activity relationships and new insights into the mechanism of the direct H₂O₂ synthesis [1].

Reference
[1] M. Selinsek, B.J. Deschner, D.E. Doronkin, T.L. Sheppard, J.-D. Grunwaldt, R. Dittmeyer, ACS Catal. 8 (2018) 2546.

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