



Contribution ID: 424

Type: Talk

Operando XAS studies of direct synthesis of H₂O₂ over Pd catalysts

Tuesday, 18 September 2018 11:30 (15 minutes)

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 auto-oxidation 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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Session Classification: Micro symposium 4

Track Classification: MS4 Innovation and industry