

## Well-defined iron sites on the silica surface: characterization and reactivity

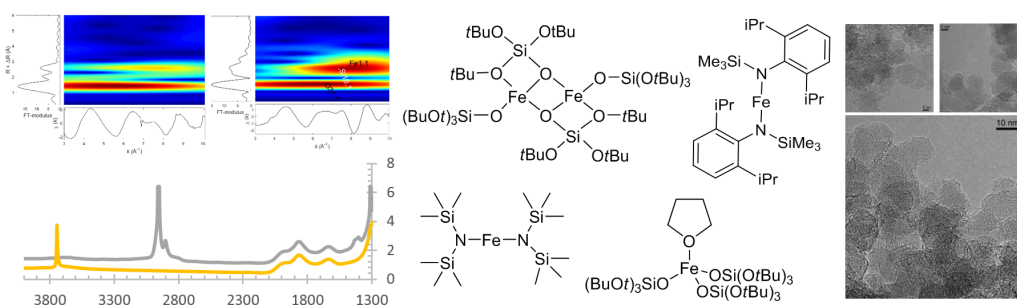
P. Šot<sup>1</sup>, D. P. Estes<sup>1</sup>, C. Copéret<sup>1\*</sup>, J. A. van Bokhoven<sup>1,2\*</sup>

<sup>1</sup>ETH Zurich, <sup>2</sup>Paul Scherrer Institute, Villigen

>Single iron (II) and iron (III) sites were successfully employed as catalysts in a variety of chemical reactions, including propane dehydrogenation,[1] oxidation of alkanes, alkenes and arenes and non-oxidative coupling of methane. [2,3] Nevertheless only very limited number of reports describe their nuclearity and reactivity on the surface. [1-5]

In this study siloxide based (e.g. iron(II) siloxide, iron(III) siloxide) and silylamide based materials (e. g. iron(II) bis(trimethylsilyl)amide, iron(II) bis(2,6-diisopropylphenyl)(trimethylsilyl)amide) were synthesized and grafted on the surface of partially dehydroxylated silica. Their structure was studied with variety of spectroscopic methods (X-ray absorption spectroscopy, infrared spectroscopy, electron paramagnetic resonance, etc) which indicate, that they preserve their original nuclearity even on the surface of the silica.

Such active sites show activities towards the non-oxidative dehydrogenation of propane, similarly to Co(II), Cr(III) and Ga(III) isolated sites.



[1] Hu, B.; Schweitzer, N. M.; Zhang, G.; Kraft, S. J.; Childers, D. J.; Lanci, M. P.; Hock, A. S. *ACS Catal.* **2015**, *5*(6), 3494-3503.

[2] Nozaki, C.; Lugmair, C. G.; Bell, A. T.; Tilley, T. D. *J. Am. Chem. Soc.* **2002**, *124*(44), 13194-13203.

[3] Guo, X.; Fang, G.; Li, G.; Ma, H.; Fan, H.; Yu, L.; Tan, D. *Science.* **2014**, *344*(6184), 616-619.

[3] Roukoss, C.; Basset, J. M.; Copéret, C.; Lucas, C.; Kuntz, E. *C. R. Chim.* **2008**, *11*(6), 620-627.

[4] Deschner, T.; Törnroos, K. W.; Anwender, R. *Inorg. Chem.* **2011**, *50*(15), 7217-7228.

[5] Holland, A. W.; Li, G.; Shahin, A. M.; Long, G. J.; Bell, A. T.; Tilley, T. D. *J. Catal.* **2005**, *235*(1), 150-163.