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Wednesday, February 16, 2011
Crowne Plaza Hotel, Somerset, New Jersey

Dr. Maria Veronica Ganduglia-Pirovano
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**“A theoretical perspective of the effect of the support in heterogeneous catalysis:
The example of vanadia catalysts for selective oxidation”**

Supported vanadium oxides (VO_x) are active in several important oxidation reactions such as the oxidative dehydrogenation of alkanes to alkenes. The strong influence of the oxide support on the reactivity is well known, but the different factors that may contribute to it and their interplay are not fully understood. Specifically, VO_x/ceria is significantly more reactive than VO_x/alumina. The difficulties in characterizing the surface structure of powder (real) catalysts and in identifying the active species under catalytic relevant conditions have strongly motivated the experimental [1, 2] and theoretical study of model catalysts [2, 3] such as VO_x on Al₂O₃ and CeO₂.

Here, I report theoretical models for alumina and ceria supported VO_x species. By combining density functional theory calculations with statistical thermodynamics, I discuss the stability of the VO_x species as function of the oxygen partial pressure, vanadia loading, and temperature. A detailed characterization of the structural, electronic and vibrational properties of these model catalysts is provided. The results are consistent with the experimental knowledge for powder catalysts and experimental model catalysts and thus help to bridge the gap between them.

Reactivity descriptors such as the energy of oxygen defect formation (which relate to the reaction energy in oxidation reactions) and the energy of hydrogenation (which relates to the energy barrier of the rate determining step) have been used to compare the catalytic activity of the different systems. These descriptors have been instrumental in elucidating the origin of the remarkably high activity of vanadia supported on ceria as compared to alumina. The effect of the ceria support is, in fact, a cooperative effect between vanadia and ceria which can be considered as a promoting effect of the vanadia species on the activity of the uncovered ceria support.

*This work has been carried out at the Humboldt-University Berlin in collaboration with J. Sauer, C. Popa, V. Brázdová, J. L. F. Da Silva, T. K. Todorova, and Y. Shimodaira.

References

[1] N. Magg, B. Immaraporn, J. B. Giorgi, T. Schroeder, M. Bäumer, J. Döbler, Z. Wu, E. Kondratenko, M. Cherian, M. Baerns, P. Stair, J. Sauer, H.-J. Freund, *J. Catal.* 226, 88 (2004).

[2] M. Baron, H. Abbott, O. Bondarchuk, D. Stacchiola, A. Uhl, S. Shaikhutdinov, H.-J. Freund, C. Popa, M. V. Ganduglia-Pirovano, J. Sauer, *Angew. Chem. Int. Ed.* 48, 8006 (2009); M. V. Ganduglia-Pirovano, C. Popa, J. Sauer, H. Abbott, A. Uhl, M. Baron, D. Stacchiola, O. Bodarchuk, S. Shaikhutdinov, and H.-J. Freund, *J. Am. Chem. Soc.* 132, 2345 (2010).

[3] V. Brázdová, M. V. Ganduglia-Pirovano, V. Simic-Milosevic, J. Sauer, *J. Phys. Chem. C* 114, 4983 (2010); T. K. Todorova, M. V. Ganduglia-Pirovano, and J. Sauer, *J. Phys. Chem. C* 111, 5141 (2007); V. Brázdová, M. V. Ganduglia-Pirovano, and J. Sauer, *J. Phys. Chem. B* 109, 23532 (2005).

Dinner is a buffet, and includes <u>a choice of beef, chicken or fish</u>		Members	\$37
		Non-members	\$45
Social Hour (Cash Bar)	6:00 PM	Students	\$17 (<i>Student Members = \$5</i>)
Dinner	7:00 PM	Retired/Post-Doc/ Unemp.	\$37 (<i>Members = \$27</i>)
Presentation	7:45 PM	Annual Dues	\$15

Deadline for dinner reservations is 2:00 p.m. Friday, February 11, 2011

Call or email Amanda Josey (973) 245-6173 (amanda.josey@basf.com) for reservations. With the exception of extreme circumstances, anyone not canceling reservations by the above deadline will be billed for dinner regardless of attendance.

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