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Characterization of Amorphous Silica Based Catalysts and Materials Using DFT Computational Methods

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Abstract

The silicate minerals make up the largest and most important class of rock-forming minerals, constituting more than 90 percent of the crust of the Earth. Silicate minerals all contain silicon and oxygen, but can contain naturally or synthetically other types of atoms. The abundance and the rich variety of crystal structures as well as their low prize make them materials of great interest in a many technological applications. One of these important SiO2 based materials/catalysts is amorphous silica.

Much of our current understanding of catalytic activity is derived from materials with well-defined structures, either molecular (i.e., homogeneous catalysts) or extended, ordered solids (i.e., surface science), and active sites in real catalysts are often assumed to closely resemble structures found in such ordered materials, at least locally. Yet many real catalysts involve amorphous materials and are much more active than their well-ordered counterparts would suggest. This implies that at least some active sites in amorphous materials are intrinsically different.

The properties are based in many cases on the way molecules interact with the silicate's surface. Since several years we investigate silicates and their role as support of transition metal oxide catalysts, but also the interaction with bio-organic, and this at different levels: from the phenomenological description of the interaction at the interface substrate-adsorbate (adsorption and self-assembling of biomolecules) to technologic applications (catalysis, ionic liquids), pharmaceutical (controlled delivery of drug molecules) and their plausible role in different scenarios in the origin of life [1-7]. For this we use the tools of quantum chemistry combined with experimental back up with the aim to improve the understanding of the complex chemical behavior of these materials.

References

(1) F. Tielens, C. Gervais, J.-F. Lambert, F. Mauri, D. Costa, Chem. Mater. 20, 3336 (2008).
(2) M.M. Islam, D. Costa, M. Calatayud, F. Tielens, J. Phys. Chem. C 113, 10740 (2009).
(3) H. Guesmi, R. Gryboś, J. Handzlik, F. Tielens, PCCP, 16, 18253 (2014).
(4) J. Handzlik, R. Gryboś and F. Tielens, J. Phys. Chem. C, 117, 8138, (2013).
(5) D.C. Tranca, A. Wojtaszek, M. Ziolek, F. Tielens, Picture, PCCP, 17, 22402 (2015).
(6) A. Wojtaszek, I. Sobczak, M. Ziolek, F. Tielens, J. Phys Chem. C 114, 9002 (2010).
(7) N. Folliet, C. Gervais, D. Costa, G. Laurent, F. Babonneau, L. Stievano, J.-F. Lambert, F. Tielens, C, 117, 4104, (2013).

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