EuroSciCon

Euroscicon Conference on

Physical Chemistry and Analytical Separation Techniques

October 08-09, 2018
Amsterdam, Netherlands

Manuel J Louwerse, J Org Inorg Chem 2018 Volume: 4
DOI: 10.21767/2472-1123-C6-017

MODELLING ION DIFFUSION OVER HYDROXYLATED SUPPORT SURFACES

Manuel J Louwerse

Debye Institute for Nanomaterials Science-Utrecht University, The Netherlands

For many processes in chemistry and in catalysis, diffusion plays an important role. Specifically, for forming nanoparticles during the preparation of solid catalysts and for sintering during their use, controlling the diffusion of metal atoms or ions is the key. The diffusion of metal atoms over the surface of metallic nanoparticles, pristine support surfaces, and hydroxylated support surfaces has been studied before by others. However, the diffusion of metal ions over (hydroxylated) support surfaces has not yet received any attention. Nonetheless, especially during catalyst preparation it is ions that diffuse, so the mobility of ions needs to be studied as well. For the diffusion of ions, everything revolves around the behaviour of counter-charges: displacements of charged ions without any charge compensation would lead to charge separation resulting in high diffusion barriers. However, co-diffusion of counter-ions is not trivial, since these are often incorporated in the hydroxylation layer and are strongly bound by hydrogen bonds. For the co-diffusion of OH^- ions, we have observed that there are two possible mechanisms: adjustments of the hydrogen bond network to allow OH^- co-diffusion, or counter-diffusion of protons, or a combination of these two mechanisms. Using density functional theory (DFT), we studied the diffusion of Cu^{2+} and Cu^+ ions over the surface of γ-alumina at varied hydration states. Apart from setting up a methodology to overcome the challenges of sampling, the many possible adjustments of the hydrogen bond network, we have found interesting trends in the balance between the two possible charge-compensation mechanisms depending on the hydration state of the surface and the charge of the metal ion. We anticipate that many of our conclusions can be translated to other metal ions and types of supports as well, based on the hydrophilicity of the support and the net charge of the metal ion involved

Biography

Manuel J Louwerse has completed his PhD from the Free University Amsterdam. He has worked as Researcher at Organon and TNO and had several postdoctoral positions at the University of Amsterdam and Utrecht University. His research focusses on the Application of Molecular Modelling in several fields of Chemistry. He has published more than 15 papers in reputed journals.

m.j.louwerse@uu.nl