In silico study of reaction mechanisms and design principles for water oxidation catalysts

Vallés Pardo, J.L.

CURRICULUM VITAE

From September 2003 until June 2008 I was a Chemistry student at the *Universitat de València*, joining during the last year the BOC-SSNMR group at Universiteit Leiden as an Erasmus student. The subject of my master work was: "*Study of a synthetic manganese catalyst for water splitting*". During this year I participated in the Honours Class "*From Solar to Fuel with Bio*".

After receiving my Master in Chemistry in September 2008, I started my PhD at the Universiteit Leiden under the supervision of Dr. Francesco Buda and Prof. Huub de Groot. During my PhD I participated in different schools and workshops, including *Theoretical Chemistry and Spectroscopy* (Han-sur-Lesse, Belgium, 2008), *Solar Biofuels from Microorganisms* (Leiden, 2009), *The Artificial Leaf* (Leiden, 2010), *Modeling Natural and Artificial Photosynthesis* (Leiden, 2011) and *The Artificial leaf* (Twente, 2012). In 2010 I have been also visiting for a period of two weeks the Physikalisch Chemisches Institut in Zürich, where I worked in the department of

Prof. Dr. Jürg Hutter learning from the developers the basics of the CP2K software. I presented my research work at various meetings and conferences, with poster presentations at *MolSim: Understanding Molecular Simulation* (Amsterdam, 2010), *Psi-K* (Berlin, 2010), *Modeling Natural and Artificial Photosynthesis* (Leiden, 2011) and *CPMD Meeting* (Barcelona, 2010); and with oral presentations at *CHAINS* (Maarsen, The Netherlands, 2011) and *HRSMC meeting* (Amsterdam, 2012).

LIST OF PUBLICATIONS

- **"Ab-initio molecular dynamics study of water oxidation reaction pathways in mono-Ru catalysts"**

J.L. Vallés-Pardo, M.C. Guijt, M. Iannuzzi, K.S. Joya, H.J.M. de Groot, F. Buda, *ChemPhysChem: a European journal of chemical physics and physical chemistry* 13 (**2012**) 140-146.

- **"Structural rearrangements and reaction intermediates in a di-Mn water oxidation catalyst"**

J.L. Vallés-Pardo, H.J.M. de Groot and F. Buda, *Physical Chemistry Chemical Physics*, 14 (**2012**) 15502-15508.

- **"Molecular Catalytic Assemblies for Electro-driven Water Splitting"**

K.S. Joya, J.L. Vallés-Pardo, Y. Faheem, T. Eisenmayer, B. Thomas, F. Buda, H.J.M. de Groot, *ChemPlusChem* (**2012**). DOI: 10.1002/cplu.201200161. *Accepted*.

- **"*In silico* prediction and thermodynamic study of novel mono-nuclear water oxidation catalysts"**

J.L. Vallés-Pardo, H.J.M. de Groot and F. Buda. (2012). *To be submitted*.