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Molecular catalytic system for efficient water splitting

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List of Publications/Patents

Patents:

Khurram Saleem Joya and Huub J.M. de Groot, Metal complex and use as multi-electron catalyst. *Netherlands Patent Application* no. 2005512, Oct., 2010.

Khurram Saleem Joya and Huub J.M. de Groot, Metal complex and use as multi-electron catalyst. *International Patent Application* no. PCT/NL2011/050673; Oct., 2011.

Publications:

- 1- K.S. Joya and H.J.M. de Groot, Electroassisted water splitting by single site half sandwiched molecular complexes anchored on the electrode surface via a tunneling barrier, *in preparation*.
- 2- K.S. Joya and H.J.M. de Groot, Rapid and efficient water oxidation by aqua induced mononuclear iridium complexes, *in preparation*.
- 3- K.S. Joya and H.J.M. de Groot, Surface enhanced electrocatalytic water splitting by single site iridium complexes, 2011, *submitted*.
- 4- K.S. Joya and H.J.M. de Groot, Biomimetic molecular water splitting catalysts for hydrogen generation. *Int J. Hydrogen Energy*, 2011, *in revision*.
- 5- K.S. Joya and H.J.M. de Groot, Molecular water oxidation catalysts with bifunctional aqua induction and proton management for a four step PCET pathway, *in preparation*.
- 6- K.S. Joya and H.J.M. de Groot, A mononuclear water splitting mimic of Photosystem-II with a four-step proton coupled electron transfer regime, 2011, *submitted*.
- 7- K.S. Joya and H.J.M. de Groot, Efficient water splitting by single site ruthenium catalyst. *Proceedings 4th European conference on chemistry and life sciences*, 2011, *submitted*.
- 8- K.S. Joya, H.J.M. de Groot and M.T.M. Koper, Rotating ring-disc electrode and surface enhanced raman spectroscopy studies of water splitting by trinuclear ruthenium catalyst adsorbed on gold, *to be submitted*.
- 9- J.L. Vallés-Pardo, M.C. Guijt, M. Iannuzzi, K.S. Joya, H.J.M. de Groot and F. Buda, Ab-initio molecular dynamics study of water oxidation reaction pathways in mono-Ru catalysts. *ChemPhysChem* 2011, *in press*.

Publications before PhD:

- 10- Y. Faheem and K.S. Joya, Phase transformation and freestanding nanoparticles formation in lead zirconate titanate derived by sol-gel. *Appl. Phys. Lett.*, 2007, 91, 063115-1 – 063115-3.
- 11- M. Amjad and K.S. Joya, Electrochemical hydrogen evolution reactions on cobalt-molybdenum electrodes. *Pak. J. Sci. Res.*, 2007, 59 (1-2), 16–21.
- 12- K.S. Joya and F. Tahira, Synthesis of zeolite 4A molecular sieves from kaolin by clay mineral conversion process. *Pak. J. Sci. Res.*, 2007, 59 (1-2), 44–48.
- 13- K.S. Joya, M. Amjad, Y. Faheem and A. Siddiq, Electrodegradation of 2-Chlorophenol at Modified Cylindrical Vitreous Carbon Electrode. *Pak. J. Sci. Res.*, 2007.
- 14- K.S. Joya, M. Amjad, Y. Faheem and S. Akhtar, Electrochemical oxidation of alkyl benzene sulfonate at modified platinum microdisk. *Pak. J. Sci. Res.*, 2007.
- 15- K.S. Joya, M. Amjad, M.A. Khurram and S. Waheed, Anodic polarization of Pb-Sb and Sn-Pb electrodes in sulphuric acid solution. *Pak. J. Sci. Res.*, 2007.
- 16- K.S. Joya, M. Amjad and S. Waheed, Investigation of corrosion rate in certain alloys used for industrial cooling water system. *J. Pak. Inst. Chem. Engg.*, Vol. XXXIV 2007.

- 17- K.S. Joya, M. Amjad and A. Siddiq, Study of various parameters involved in electrochemical machining of mild steel in sodium nitrate and sodium chloride electrolytes. *J. Pak. Inst. Chem. Engg.*, Vol. XXXIV 2007.
- 18- M. Amjad and K.S. Joya, Effect of silver as an alloying additive on the anodic behaviour of lead dioxide electrode. *Pak. J. Sci.*, 2006, 58 (3-4), 79–83.
- 19- K.S. Joya, M. Amjad and A. Khurram, Comparative study on the anodic oxidation of normal butanol at Pb, Pb-Sb, Pb-Sn And Sn-Pb alloy electrodes. *Pak. J. Sci.*, 2006, 58 (3-4), 84–88.
- 20- K.S. Joya, M. Amjad and A. Sadia, Linear sweep voltammetry for electrochemical oxidation of alkyl benzene sulfonate in waste water. *Pak. J. Sci., Res.* 2006, 58 (3-4), 26–30.
- 21- K.S. Joya and M. Amjad, A comparative study on the anodic behaviour of arsenic and bismuth doped lead dioxide electrodes. *Pak. J. Sci. Res.*, 2005, 57 (3-4), 104–108.
- 22- M. Amjad, K.S. Joya and U.A. Bilal, Electrochemical oxidation on PbO₂ electrodes electrodeposited from Cs⁺ containing Pb⁺⁺ electrolytes. *Pak. J. Sci. Res.*, 2005, 57 (3-4), 159–162.
- 23- K.S. Joya, M. Amjad and Asif Ali, Investigation of oxidation processes at different Pb-Sb alloy anodes. *J. Pak. Inst. Chem. Engg.*, 2004, 32, 41–46.
- 24- M. Amjad and K.S. Joya, Anodic behaviour of antimony and arsenic doped lead dioxide electrodes. *J. Pak. Inst. Chem. Engg.*, 2003, 32 (1-4), 43–46.

Curriculum Vitae

I, **Khurram Saleem Joya**, the author of this dissertation, was born on 5th of January, 1979 in Lahore, Pakistan. While growing in a scientific family, I inherited interest and curiosity for science from my parents, especially from my Father. At the age of 8, I passed a junior school test and entered fourth class in 1987. After spending one and a half year at Govt. Muslim Model Junior School, I moved to the High School and passed my SSC/Matric. I was 14 when I got admission in Govt. Forman Christian (F.C.) College Lahore, and obtained my HSSC/FSc diploma in 1996. After this, I joined Govt. College (G.C.) Lahore, and did my graduation with Botany/Zoology/Chemistry combination, and obtained my BSc degree, in 1998. At the age of 19, I entered the Faculty of Chemistry of the University of Engineering and Technology (UET), Lahore, and got my MSc in Applied Chemistry in January, 2001. During my MSc research, I worked with Prof. Dr. M. Amjad on an electrochemistry project and developed new doping for PbO_x matrix for electro-oxidation of alkanols.



In February 2001, I joined the same department as a faculty member and became a regular Lecturer in Chemistry at UET, Lahore in December 2001. While continuing my teaching and research at UET, Lahore, I also obtained my M.Phil in Applied Chemistry in 2006 and did my research on Zeolite Molecular Sieves, Synthesis and Application, with Prof. Dr. F. Tahira. In the meantime, I also supervised six MSc research projects dealing with Electrochemistry, Electrochemical Machining (ECM), Zeolites and Corrosion Science, which resulted in 6 MSc theses and 9 publications. My early research in Pakistan has generated more than 15 research papers in local journals. During my professional carrier at UET, Lahore, I was also involved in many activities, such as: Proctoral Board, Library Committee, Tutorial Board and Guidance Bureau (2003-2007), elected member of UET Syndicate, Senate, Admission Cell (2004-2007), Head Sports, Tour, Functions Committee (Chemistry Department) (2002-2007).

In early 2007, I was granted with the HEC (Higher Education Commission) Pakistan, overseas PhD Scholarship and in September 2007, I started my PhD with Prof. Dr. H.J.M. de Groot (SSNMR) and Prof. Dr. M.T.M. Koper (CASC) at Leiden Institute of Chemistry, Leiden University, The Netherlands. While working on the water splitting project that is the

topic of the research in this thesis, I discovered a new class of oxygen evolving catalysts in 2010, and this invention has been filed as a Patent Application as well.

During my four years of PhD, I participated in various international and local conferences, courses and schools, where I presented my work. Among more than 20 meetings/conferences I have attended, the most important include: *NCCC IX* (2008), *XI* (2010) and *XII* (2011), and *Annual HRSMC Symposiums* (2008-2011) The Netherlands; *Solar-H2 Meeting*, 2008, Bochum, Germany; *Solar Fuels/Energy Meeting*, 2008, Berlin, Germany; *59th ISE Annual Meeting*, 2008, Seville, Spain; *International Conference Molecular Science for Solar Fuels*, 2009, Sigtuna, Sweden, *ISACS 2011: Challenges in Renewable Energy*, 2011, MIT, Boston, USA; *Photosynthesis Research for Sustainability*, 2011, Baku, Azerbaijan (Invited speaker); *Towards Global Artificial Photosynthesis, Energy, Nanochemistry & Governance*, 2011, Lord Howe Island, Australia (Invited plenary lecture); *4ECCLS*, 2011, Budapest, Hungary and *SolarFuelsTandem Meeting*, 2011, Mülheim, Germany.

I have also participated in *Solar-H2 Summer School*, 2008, Uppsala University, Sweden, and *EBSA Biophysics Course on Solar Energy - Biological and Biomimetic Solutions*, 2011, Szeged, Hungary. In 2009, I obtained two consecutive LUF grants from Leiden University and conducted two research internships in the group of Prof. Dr. J.S. Siegel at Institute of Organic Chemistry, University of Zürich, Switzerland. I was also invited for a practical demonstration of my catalytic water splitting system at the *BioSolar Cells (TBSC) Project Meeting*, 2011, Wageningen, The Netherlands.

Besides this, I joined Pakistan Tehreek-e-Insaf Holland Chapter (PTI-Holland) in 2010 and served as General Secretary and currently Vice President of the party.

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It is important to realize that I would have never arrived at this point without the continuous educational support of many people, all my School and College teachers, who nourished me with knowledge and guidance. My university teachers showed me the beauty and wonders of science, in particular chemistry that has inspired me to do research in this field. It is worth mentioning the input of my MSc research supervisor Prof. Dr. Muhammad Amjad and Prof. Dr. Fazeelat Tahira during my MPhil project, for giving me a broader spectrum of research and confidence to explore new things in science and chemistry. My kind regards to Lt. Gen. (R) M. Akram Khan, vice chancellor University of Engineering and Technology (UET), Lahore for his interest in my PhD progress and the partial ownership of our Patent. The bold and steady steps taken by our ex-president Gen. Pervez Musharraf for the development of science and technology in Pakistan and for establishing the HEC (Higher Education Commission) are highly acknowledged. My sincere gratefulness to HEC for the overseas PhD scholarship and financial support for my four years stay in Netherlands.

I would like to mention my colleagues in the SSNMR group, our secretary Liesbeth van der Velden, members of CASC, MCBIM and Leiden University for their collaboration during my PhD research. I am very happy that Prof. Dr. Gijs A. van der Marel facilitated me in the organic synthesis lab and Dr. Rob van der Steen (LIC/Buchem B.V) for helping my students. I appreciate the useful discussions with Prof. Dr. Jan Reedijk, Dr. Francesco Buda, Dr. Partik Gamez and Dr. Sylvestre Bonnet during my work. Fons Lefeber and Cees Erkelens are acknowledged for their help in NMR measurements. Working with Dr. Reza Fallahpour at University of Zürich, Switzerland, was a good experimental experience for my initial learning of the polypyridyl compounds and heterocyclic synthesis. I also appreciate help of Michiel Cramwinkel and Art Bos for preparation and filing patent applications and suggestions of K.C. Daniël and Paul Hedges.

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Working in the laboratory has definitely become easier due to a nice and relaxing social environment and communication with special people: Nauman Javed (FCU Lahore), Dr. Umar Farooq Rizvi/Kalia (Lahore), M. Shahzad Yousaf/Sundar-Sundi (Gujranwala), Dr. Irfan Ashiq/Paa-G (Lahore), M. Farooq, M. Raza and Irfan Jajja (London, UK), Bilal Ahmad Farooqi (Islamabad), Frid ullah momin (Copenhagen, Denmark), Shahid Akram Javed (Sahiwal), Ahmad Raza, Masood and M.P. Sajid (Lahore), Majeed Ullah Niazi (Mianwali), Imran Qaisar (Sheikhupura). I value the friendship of Abubakar (Saudi Arabia), M. Fahad (Dubai), Kashif Ali Khan/Rook (UET, Lahore) and Ehsan Ullah/Cheunti (Boston, USA).

Faisal and Sarah Chaudhary (Canada), Ali and Rowida Marashdeh, M. Miqiyaas and Kinza and Mahmood (Leiden, The Netherlands) always had a kind attitude towards me and my family, and their hospitality and openness is highly commendable. Muhammad Hissi, Khaled and Taleb (Leiden, The Netherlands) were nice companions and gym-mates. The officials of Pakistan Tehreek-e-Insaf Holland Chapter (PTI-Holland), Dr. Gulsher Khaliq, Baber Bhatti, Bilal Ahmad, Ghulam Hussain and Rizwan Akhtar for gave me respect and trust, and I appreciate the optimistic thinking we have for the better future of Pakistan.

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اپنے والدین کے لیے لامحدود شکر یہ، عزت، محبت اور احساسات کے اظہار کے لیے میرے پاس الفاظ نہیں ہیں میں کہنا چاہتا ہوں کہ آپ کی مسلسل دعاؤں محبت اور دیکھ بھال کا بہت شکر گزار ہوں، میرے والد ڈاکٹر عبداللہ عاصم ایک بہترین شخصیت، کہانی سنانے والے اور ٹیکنالوجی میں بہترین مہارت رکھتے ہیں، مجھے اپنے والد سے علوم ہوا کہ سائنسدان ایک مفکر اور بہترین ممبر کرنے والے انسان ہوتے ہیں، میرے والد جو نیا گھر کے سربراہ ہیں لیکن میری والدہ ایک عظیم والدہ ہیں اور وہ ہی ہمارے گھر کا دل ہیں، امی جی میں ہمیشہ آپ کی گرم ہوشی، پیار، صبر اور محبت یاد کرتا ہوں، جس کے ساتھ آپ نے میری پرورش کی ہے، پیارے امی جی اور ابو جی میں آپ دونوں سے بہت پیار کرتا ہوں اور آپ کی لمبی عمر اور اچھی صحت کے لیے دعا گو ہوں، آمین

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Khurram Saleem Joya

2011, Leiden, The Netherlands