


# Alupe University College Staff Profile

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<b>1. Name:</b>	<p><i>Dr MAGERO Denis</i>  School of Science  Department of Chemistry and Biochemistry</p>
<b>2. Passport photo:</b>	
<b>4. Biography:</b>	<p>Currently staff at Alupe University College. Denis is a PhD holder in Molecular and Structural Chemistry with a special interest in computational chemistry and transition metal complexes. He is actively involved in teaching, research and administration in the university. He is working on a collaborative project on materials for energy storage with collaborators from University of Grenoble. The work has earned him a postdoctoral study in France. He is also engaged in the development of computational chemistry in Africa under the African School on Electronic Structure and Methods (ASESMA). See links for further information.</p>
<b>5. Academic Qualifications:</b>	<p>Postdoctorate (Universite of Grenoble Alpes), 2019  Finding the minimum energy passes on the triplet energy surface of ruthenium polypyridine complexes over which the reactions are most likely to deactivate</p> <p>Ph.D (Molecular and Structural Chemistry), 2017, Grenoble Alpes University (France).  Thesis: “Partial Density of States Ligand Field Theory (PDOS-LFT): Recovering a LFT-Like Picture and Application to Photoproperties of Ruthenium Polypyridine Complexes.” <a href="https://tel.archives-ouvertes.fr/tel-01712697">https://tel.archives-ouvertes.fr/tel-01712697</a></p> <p>M.Sc (Physical Chemistry), 2013, University of Eldoret.  Thesis: “<i>ab-initio</i> Studies of Magnesium Hydride and Lithium Hydride for Hydrogen Storage Applications: A Density Functional Theory Study.”</p> <p>Environmental Impact Assessment and Environmental Audit Course, 2009 Moi University.  Registered with National Environment Management Authority (NEMA) as an associate expert.</p>

	B.Sc (Chemistry), 2009, Moi University.
<b>6. Research Interests:</b>	Inorganic and Physical Chemistry (Computational Chemistry) as well as experimental work. Simulation and study of energy storage materials using <i>ab-initio</i> methods and other new materials that may contribute to the improvement of energy efficiency. Currently, material science is also an area of interest. Projects currently ongoing include energy barrier search for transition metal complexes, excitonic effects on spectra of parallel stacked ethylene, CO <sub>2</sub> photoreduction at nanostructured copper oxides surfaces and alloying Cu for enhanced CO <sub>2</sub> electro-reduction and product selectivity. Some of the work is being in collaboration with researchers from Moi University, University of Eldoret and Universite of Grenoble Alpes.
<b>7. Publications :</b>	<p style="text-align: center;"><b>o Conferences</b></p> <p>Summer school/workshop on Computational Chemistry. University of Mauritius, Mauritius, 29 September to 12 October, 2019.</p> <p>The 5<sup>th</sup> African School on Electronic Structure Methods and Applications (ASESMA 2018). Addis Ababa Science and Technology University (AASTU), Addis Ababa, ETHIOPIA. 22<sup>nd</sup> October-3<sup>rd</sup> November, 2018.</p> <p>Computational Modelling and Materials Science (CMMS) Workshop. Masinde Muliro University of Science and Technology, Kakamega. 6-7<sup>th</sup> July, 2017.</p> <p>The 4<sup>th</sup> African School on Electronic Structure Methods and Applications (ASESMA 2016). University of Ghana, Accra, GHANA. 13-24<sup>th</sup> June, 2016.</p> <p>The 3<sup>rd</sup> African School on Electronic Structure Methods and Applications (ASESMA 2015). University of the Witwatersrand, Johannesburg, SOUTH AFRICA. 19-30<sup>th</sup> Jan, 2015.</p> <p>The 2<sup>nd</sup> Science, Technology and Innovation week organized by the National Commission for Science, technology and innovation. Kenyatta International Conference Centre (K.I.C.C) Nairobi, 13<sup>th</sup> to 17<sup>th</sup> May, 2013.</p> <p>The 1<sup>st</sup> Young Scientist Material Science and Solar Energy Network for Eastern and Southern Africa (MSSEESA), Conference on Material Science and Solar Cell Technology. United Kenya Club, Nairobi, 28<sup>th</sup> to 29<sup>th</sup> November, 2013.</p> <p>Quantum Espresso and Quantum Monte Carlo Workshop. Chepkoilel University College (Moi University), KENYA. February, 2012.</p> <p>The 2<sup>nd</sup> African School on Electronic Structure Methods and Applications (ASESMA 2012). Chepkoilel University College (Moi University), KENYA. 28<sup>th</sup> May to 8<sup>th</sup> June, 2012.</p>

	<p>Nanotechnology and Materials Science Conference. Kenyatta University, KENYA. 18<sup>th</sup> July to 20<sup>th</sup> July, 2012.</p> <p>School on Numerical Methods for Materials Science Related to Renewable Energy Applications. International Centre for Theoretical Physics, Trieste, ITALY. 26<sup>th</sup> to 30<sup>th</sup> November, 2012.</p> <p style="text-align: center;"><b>o Publications</b></p> <p>Denis Magero, Mark E. Casida, George Amolo, Nicholas Makau and Lusweti Kituyi. Partial Density of States Ligand Field Theory (PDOS-LFT): Recovering a LFT-Like Picture and Application to Photoproperties of Ruthenium Polypyridine Complexes. <i>J. Photoch. Photobio. A, Volume 348, 2017, Pages 305-325</i>, <a href="https://doi.org/10.1016/j.jphotochem.2017.07.037">https://doi.org/10.1016/j.jphotochem.2017.07.037</a>.</p> <p>Magero Denis, Lusweti Kituyi, Makau Nicholas and Amolo George. Materials for the Hydrogen Energy Economy: Magnesium Hydride (MgH<sub>2</sub>) and Lithium Hydride (LiH). <i>Kenya J. Sci. Tech. Inn. Vol 5(2015): 95-103</i>.</p> <p style="text-align: center;"><b>o Conference Papers</b></p> <p>Magero Denis, Makau Nicholas, Amolo George and Lusweti Kituyi. ab-initio studies of Lithium Hydride and Magnesium Hydride for hydrogen storage applications. The Nanotechnology and Materials Science Conference, Kenyatta University, 18<sup>th</sup> to 20<sup>th</sup> July, 2012.</p> <p>Magero Denis, Lusweti Kituyi, Makau Nicholas and Amolo George. Materials for the Hydrogen Energy Economy: Magnesium Hydride (MgH<sub>2</sub>) and Lithium Hydride (LiH). The Second National Science, Technology and Innovation Week, 13<sup>th</sup> -17<sup>th</sup> May 2013.</p> <p>Magero D., Makau N. W., Amolo G. O., Lutta S., Okoth M. D. O., Mwabora J. M., Musembi R. J., Maghanga, C. M., and Gateru R. Hydrogen as an alternative fuel: An ab-initio study of Lithium Hydride and Magnesium Hydride. 1st Young Scientist Material Science and Solar Energy Network for Eastern and Southern Africa (MSSEESA), Conference on Material Science and Solar Cell Technology. United Kenya Club, Nairobi, 28<sup>th</sup> to 29<sup>th</sup> November, 2013.</p>
<p><b>8. Classes you teach:</b></p>	<p>CHE 110: Fundamentals of Chemistry  CHE 112: Introduction to Analytical Chemistry  CHE 103: Introduction to Thermodynamics and Kinetics  CHE 104: Organic Chemistry I  CHE 210: Atomic Structure and Bonding  CHE 201: Chemical Analysis and Structure Determination  CHE 310: Chemistry of the S-and P- Block Elements  CHE 317: Electrochemistry  CHE 304E: Surface and Colloid Chemistry</p>

<b>9. Other relevant links:</b>	<a href="https://www.researchgate.net/profile/Denis_Magero">https://www.researchgate.net/profile/Denis_Magero</a> <a href="https://arxiv.org/abs/1707.03665">https://arxiv.org/abs/1707.03665</a> <a href="https://scholar.google.com/citations?user=RUZYCA0AAAAJ&amp;hl=en">https://scholar.google.com/citations?user=RUZYCA0AAAAJ&amp;hl=en</a> <a href="https://sites.google.com/site/markcasida/home/theses">https://sites.google.com/site/markcasida/home/theses</a> <a href="https://www.theses.fr/224319094">https://www.theses.fr/224319094</a> <a href="https://tel.archives-ouvertes.fr/tel-01712697/">https://tel.archives-ouvertes.fr/tel-01712697/</a> <a href="http://mcc.illinois.edu/workshops/electronicstructure/2019/Talks/ES2019_Martin.pdf">http://mcc.illinois.edu/workshops/electronicstructure/2019/Talks/ES2019_Martin.pdf</a> <a href="https://sites.google.com/site/asesmasite/people/kenya-2012/participants">https://sites.google.com/site/asesmasite/people/kenya-2012/participants</a> <a href="https://sites.google.com/site/asesma2015/names-faces/tutors">https://sites.google.com/site/asesma2015/names-faces/tutors</a>
<b>10. Official Contact Details:</b>	<ul style="list-style-type: none"> <li>• Email: <a href="mailto:dmagero@auc.ac.ke">dmagero@auc.ac.ke</a>, <a href="mailto:magerode@gmail.com">magerode@gmail.com</a></li> <li>• Telephone number(s): +254 724 73 74 54</li> </ul>