

CURRICULUM VITAE

Carlos Moyses Araujo, Ph.D

moyses.araujo@physics.uu.se

Phone: + 46 73 514 0739

Work address

Department of Physics and Astronomy
Uppsala University
Box 516
SE-751 20 Uppsala, SWEDEN

I. Appointment

2012 – present: Forskare
Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Sweden.

II. Professional preparation

2011 – 2012: Postdoctoral Researcher
Yale Climate and Energy Institute and Dept. of Chemistry, Yale University, USA.

Investigations in clean and renewable energy systems, with focus on water splitting and virtual hydrogen storage reactions. Selected publication: (i) Energy & Environmental Science (Impact factor: 20.52) 5, 9534 (2012); (ii) J. Phys. Chem. Lett. (Impact factor: 7.45) 4, 745 (2013).

2009 – 2010: Postdoctoral Researcher
Dept. of Theoretical Chemistry, Royal Institute of Technology (KTH), Sweden.

Investigation of metal coordination complexes for water oxidation reaction, with focus on homogeneous catalysis problem. Selected publication: Proc. Natl. Acad. Sci. USA (Impact factor: 9.67) 109, 15584 (2012).

2008 – 2009: Postdoctoral Researcher
Dept. of Materials Science and Engineering, Royal Institute of Technology (KTH), Sweden.

Investigation of magnetism on non-magnetic and amorphous materials. Selected publications: (i) Appl. Phys. Lett. (Impact factor: 3.30) 96, 232505 (2010); (ii) Scientific Reports (Impact factor: 5.57) 4, 4684 (2014).

2008: PhD in Physics with specialization in condensed matter physics
Department of Physics and Astronomy, Uppsala University, Sweden.

Thesis title: Hydrogen Storage Materials: Design, Catalysis, Thermodynamics, Structure and Optics.

2002: Master in Physics
Institute of Physics, Federal University of Bahia, Brazil

Thesis title: Contributions on the study of electronic structure of semiconductors: bulk and heterostructures.

1999: Bachelor
Institute of Physics, Federal University of Bahia, Brazil.

III. Prizes and Awards

2014 **Young Researcher Grant** from the Swedish Research Council.

2013 Nominated by President of KTH to the Wallenberg Academy Fellows.

2011 **Postdoctoral Position from the Yale Climate and Energy Institute (YCEI)**, at Yale University, where only four projects were granted out of forty nominees (10% of success rate).

2010 **Benzelius Prize**, awarded by the Royal Society of Sciences in Uppsala, which is the oldest Academy of Science in Sweden.

2008 **The Bjurzon's Premium**, a prestigious recognition of PhD theses in the Faculty of Science and Technology at Uppsala University.

2009 **Ångström Premium**, for excellence in research, awarded by the Department of Physics and Astronomy at Uppsala University.

2009 **Postdoctoral position from the Swedish Research Council**

IV. Granted Projects

2015 – 2018 Young Researcher Grant from Swedish Research Council (**PI**)
Title: **Advanced Hybrid Materials for High-Energy Density Storage: Fundamentals and Design** – 3,600,000 SEK for the period of four years.

2015 – 2016 Joint grant from CAPES (Brazil) – STINT (Sweden) (**Co-applicant**)
Title: **Aqueous interfaces: Molecular perspectives on climate change and sustainable energy production** – 750,000 SEK for the period of two years.

2015 – 2018 Research grant from Swedish Energy Agency (**Co-applicant**)
Title: **Progression Towards Lithium Electrodes for EV and HEV Batteries** – 3,960,000 SEK for a period of four years.

2014 – 2016 Research grant from Swedish Research Council through the program “Swedish Research Links” (**PI**) - International Collaboration with Brazil.
Title: **Advanced Nanostructured Materials for Efficient PEM Fuel Cell** – 750,000 SEK.

2013 – 2015 Research grant from Swedish Research Council through the program “Swedish Research Links” (**Principal Investigator**) - International Collaboration with Colombia.
Title: **Atomistic Modeling of Advanced Materials for CO₂ Reduction: A Promising Approach for Conversion and Storage of Solar Energy** – 750,000 SEK.

2011 – 2013 Postdoctoral Position from Yale Climate and Energy Institute, Yale University, USA.
Title: **Catalysts for Green Energy: Solar Fuel Production and Virtual Hydrogen Storage** - US\$ 120,000 for a period of two years.

2009 – 2010 Postdoctoral Position from Swedish Research Council
Title: **Nanostructured semiconductors for photo-electrochemical hydrogen** – 750,000 SEK for a period of two years.

V. Supervision of graduate students and postdoctoral fellows

- **Main supervisor for PhD student:**

Giane Damas (Department of Physics and Astronomy, UU, started on September 2014).

José Luis Silva (Department of Physics and Astronomy, UU, starts on February 2016)

- **Main supervisor for visiting PhD student:**

William Espinosa (Department of Physics and Astronomy, UU, for three months, 2015).

Andrés Uribe (Department of Physics and Astronomy, UU, for three months, 2015).

- **Co-supervisor for PhD student:**

Mahsa Ebadi (Department of Chemistry, UU, started on April 2015).

- **Assistant supervisor for postdoc:**

Puspamitra Panigrahi (Department of Physics and Astronomy, UU, 2012-2014).

- **Mentor for PhD students:**

Andreas Blomqvist (UU-2010), Pornjuk Srepusharawoot (UU-2010), Jawad Nisar (UU-2012) and Cecilia Århammar (KTH-2010).

VI. Teaching activities and pedagogical education

2015 – Statistical Mechanics, Department of Physics and Astronomy, Uppsala University, Sweden (Bachelor students level, 5 credits).

2015 – Symmetry and Group Theory Course, Department of Physics and Astronomy, Uppsala University, Sweden (MSc/PhD students level, 5 credits)

2012 – 2014 Solid State Theory Course, Department of Physics and Astronomy, Uppsala University, Sweden (MSc/PhD students level, 10 credits).

2012 – Attended “Doctoral Supervisor Training Course” within the Faculty of Science and Technology, Uppsala University.

2013 – Attended “Teacher Training Course” full time five weeks course, Uppsala University.

VII. Invited Presentations

2015 – *Brazil-Sweden Collaborative Networks to Address Green-Energy Issues*, **Invited talk, Brazil-Sweden Workshop on Frontier of Science and Education**, October 16th, FAPESP, São Paulo, Brazil.

2015 – *Atomic-scale Design of Photo-electrodes for Solar Fuel Production: Insights from First-principles Theory*, **Invited Talk, XIV Brazil Materials Research Society (MRS) Meeting**, September 27th – October 1st, Rio de Janeiro, Brazil.

2015 – *Assessing Photocatalytic Power of Semiconductors from Quasi-Particle and Time-dependent Density Functional Theory*, **Invited Talk, Workshop on Promising Approaches for Conversion and Storage of Solar Energy**, October 8-9, Medellin, Colombia.

2015 – *Solar Energy Conversion to Synthetic Fuels*, **Invited Talk, Kickoff Meeting of the CAPES-STINT collaboration “Aqueous interfaces: Molecular perspectives on climate change and sustainable energy production”**, August 9-12, Maresias, São Paulo, Brazil.

2015 – *First-principles Design of Organic Compounds for Sustainable Energy Storage*, **Invited colloquium**, École Normale Supérieure de Lyon, March 18th, Lyon, France.

<http://www.ens-lyon.fr/CHIMIE/actualites/seminaires/dr-c-araju>

2014 – *First-principles Study of Energy Materials*, **Invited Seminar, Universidad de Antioquia**, Medellin, Colombia.

2013 – *Materials for Energy Relevant Applications: A theoretical Expose*, **Invited Talk**, Swedish Excellence Seminar, November 11th, São Paulo, Brazil.

2012 – *Solar energy conversion and storage – a bridge across the disciplines of physics and chemistry*, **Invited lecture**, Winter School, Salvador, Bahia, Brazil.

2012 - *Clean Energy Matrix from Artificial Photosynthesis*, **Invited lecture**, Science Academy of Bahia, Salvador, Brazil.

2010 - *Hydrogen economy: Production, storage and usage*, **Invited seminar**,

Department of Physics, **Universidad Austral de Chile**, Chile.

2009 - *Ionic transport in crystalline solids via first-principles theory*, **Invited seminar**, Department of Physics, **Federal University of Bahia**, Brazil.

2009 - *Hydrogen economy: Storage and Production*, **Invited lecture** in the course “Energy Relevant Materials” given at **Uppsala University**, Sweden.

2009 - *Computational studies of hydrogen storage materials*, **Invited seminar** at Department of Theoretical Chemistry, School of Biotechnology, **Royal Institute of Technology (KTH)**, Sweden.

2009 - *First-principles investigation of hydrogen storage materials*, **Invited colloquium**, Department of Physics, **National University of Singapore**, Singapore.

2009 - *Superionicity in Li-N-H systems*, **Invited seminar**, Department of Physics, **Virginia Commonwealth University (VCU)**, Richmond, USA.

2008 - *Nanotechnology for Sustainable Energy*, **Invited talk**, **BAHIATEC – International Symposium of Innovation**, Salvador, Bahia, Brazil.

2007 - *Hydrogen Storage in Li-Mg-N-H systems*, **Invited talk**, **Swedish-Brazilian Workshop on Advanced Functional Materials**, Salvador, Bahia, Brazil.

2007 - *First-principles investigation of structural properties of Li_2NH and $\text{Li}_2\text{Mg}(\text{NH})_2$ and their applications for hydrogen storage* **Invited talk**, **International Symposium on Hydrogen Storage**, Miami, USA.

VIII. Publication List

~1,300 citations, **H-index=18** (web of science)/ 1,500 citations, **H-index=19** (google scholar)

80. Martin Walbrühl, Andreas Blomqvist, Pavel Korzhavyi, C. Moyses Araujo, *Surface Gradients in Cemented Carbides from First-Principles-Based Multiscale Modeling: Relevance of Atomic Diffusion in Liquid Co* **Acta Materialia** (Submitted).

79. S. Renault, V. Mihali, C. Moyses Araujo, A. Grigoriev, K. Edstrom, D. Brandell, *Super-lithiation of Organic Electrode Materials: The Case of Dilithium benzenedipropiolate* **Chemistry of Materials** (Under review).

78. J. Gonzalez Moya, Y. Garcia-Basabe, M. L. Rocco, M. Pereira, J. Princival, L. Almeida, C. Moyses Araujo, D. David, A. Ferreira da Silva, G. Machado, *TiO₂ Nanotubes Sensitized with CdS Quantum Dots via an In Situ Hydrothermal Route: A CdS Size Effect Study on the Photocatalytic Hydrogen Production*, **Nanotechnology** (Submitted).

77. M. P. Rainka, C. Moyses Araujo, D. L. Simone, S. J. Konezny, A. J. Peters, V. S. Batista and G. L. Soloveichik, *First Oxidation Potentials of Model Fuels for Regenerative Organic Fuel Cell/Flow Battery: Theory and Experiment*, **In Manuscript**.

76. R. Sanchez-de-Armas, B. Brena, I. Rivalta and C. Moyses Araujo, *Soft X-ray Spectroscopic Properties of Ruthenium Complex Catalyst under CO₂ Electrochemical Reduction Conditions: A First-Principles Study* **J. Phys. Chem. C** **119**, 22899 (2015).

75. J. M. Osorio-Guillen, W. Espinosa and C. Moyses Araujo, *Assessing Photocatalytic Power of Graphitic Carbon Nitride from Quasi-Particle Theory* **Journal of Chemical Physics** **143**, 094705 (2015).

74. Shi Tang, Jonas Mindemark, C. Moyses Araujo, Daniel Brandell and Ludvig Edman, *Identifying Key Properties of Electrolytes for Light-Emitting Electrochemical Cells*, **Chemistry of Materials** **26**, 5083 (2014).

73. P. Panigrahi, C. Moyses Araujo, T. Hussien and Rajeev Ahuja, *Crafting Ferromagnetism at Mn doped MgO Surface with p-type Defects*, **Science and Technology of Advanced Materials** **15**, 035008 (2014).

72. P. Panigrahi, T. Hussain, C. Moyses Araujo and R. Ahuja, *Hole Induced Jahn-Teller Distortion Ensuing Ferromagnetism in Mn-MgO; Bulk, Surface and One dimensional structures*, **J. Phys.: Condensed Matter** **26**, 265801 (2014).

71. B. Wang, C. Århammar, X. Jiang, C. Moyses Araujo and R. Ahuja, *A comparison between hybrid functional, GW approach and the Bethe Salpether equation: Optical properties of high pressure phases of TiO₂*, **Science of Advanced Materials** **6**, 1170 (2014).

70. C. Moyses Araujo, Sandeep Nagar, Muhammad Ramzan, R. Shukla, O.D. Jayakumar, Yi-Sheng Liu, Jeng-Lung, Chinglin Chang, Andreas Blomqvist, Raquel Lizarraga, Erik Holmstrom, Lyubov Belova, A.K. Tyagi, Jinghua Guo, R. Ahuja, K.V. Rao, *Disorder-induced Room Temperature Ferromagnetism in Chromite Thin Films*, **Nature-Scientific Reports** **4**, 4684 (2014).

69. C. G. Almeida, R. B. Araujo, R. G. Yoshimura, A. Mascarenhas, A. Ferreira da Silva, C. Moyses Araujo, Luciana A. Silva, *Photocatalytic hydrogen production with visible light over Mo and Cr-doped BiNb(Ta)O₄*, **Int. J. Hyd. Energy** **39**, 1220 (2014).

* I have designed and coordinated this project together with Prof. Silva.

68. B. Wang, J. Nisar, C. G. Almeida, A. J. S. Mascarenhas, L. A. Silva, D. G. F. David, P. Bargiela, C. Moyses Araujo, R. Ahuja, A. Ferreira da Silva, *Optical and electronic properties of nanosized BiTaO₄ and BiNbO₄ photocatalysts: Experiment and theory*, **Phys. Status Solidi B** **251**, 1034 (2014).

67. Y. G. Li, Y. L. Li, C. Moyses Araujo, W. Luo, R. Ahuja, *Single-layer MoS₂ as an efficient photocatalyst*, **Catalysis Science and Technology** **3**, 2214 (2013).

66. M. Z. Ertem, S. J. Konezny, C. Moyses Araujo, and V. S. Batista, *Functional Role of Pyridinium during Aqueous Electrochemical Reduction of CO₂ on Pt(111)*, **J. Phys. Chem. Lett.** **4**, 745 (2013).

65. C. Moyses Araujo, D. L. Simone, S. J. Konezny, A. Shim, R. H. Crabtree, G. L. Soloveichik and V. S. Batista, *Fuel selection for regenerative organic fuel cell/flow battery: thermodynamics consideration*, **Energy & Environmental Science** **5**, 9534 (2012).

64.* L. Duan, C. Moyses Araujo, M. Ahlquist, and L. Sun, Highly Efficient and Robust Molecular Ruthenium Catalysts for Water Oxidation, **Proceedings of the National Academy of Sciences of USA (PNAS)** **109**, 15584 (2012).

*I am the first-author from the theory team.

63. C. Moyses Araujo, M. Doherty, S. J. Konezny, O. R. Luca, A. Usyatinsky, G. L. Soloveichik, R. H. Crabtree, and V. S. Batista, *Tuning Electrochemical Properties of bis(imino)pyridine cobalt complex: an experimental and theoretical study involving solvent and ligand effects*, **Dalton Trans.** **41**, 3562 (2012).

62. S. Lebegue, C. Moyses Araujo, D. Y. Kim, M. Ramzan, H-K. Mao, and R. Ahuja, Semi-metallic dense hydrogen above 260 GPa, **Proceedings of the National Academy of Sciences of USA (PNAS)** **109**, 9766 (2012).

61. J. Nisar, B. Wang, C. Moyses Araujo, A. F. da Silva, Tae Won Kang, Rajeev Ahuja, *Band gap engineering by anion doping in the photocatalyst BiTaO₄: First-principles calculations*, **Int. J. Hyd. Energy** **37**, 3014 (2012).

60. T. Kaewmaraya, B. Pathak, C. Moyses Araujo, A. da Rosa, R. Ahuja, *Water adsorption on ZnO(1010): The role of intrinsic defects*, **Europhys. Lett.** **97**, 27013 (2012).

59. W. Li, L. Miao, R. H. Scheicher, Z. Xiong, G. Wu, C. Moyses Araujo, A. Blomqvist, R. Ahuja, Y. P. Feng, and P. Chen, *Li-Na ternary amidoborane for hydrogen storage: experimental and first-principles study*, **Dalton Trans.** **41**, 4754 (2012).

58. J. Nisar, B. Wang, C. Moyses Araujo, A. Ferreira da Silva, T. W. Kang, R. Ahuja, *Band gap engineering by anion doping in the photocatalyst BiTaO₄: First-principles calculations*, **Int. J. Hyd. Energy** **37**, 3014 (2012).

57. Raquel Lizarraga, Muhammad Ramzan, C. Moyses Araujo, Andreas Blomqvist, Rajeev Ahuja, and Erik Holmstrom, *Structural characterization of amorphous YCrO₃ from first principles*, **Europhys. Lett.** **99**, 57010 (2012).

56. Z. Qian, M. S. Hudson, H. Raghubanshi, R. Scheicher, B. Pathak, C. Moyses Araujo, A. Blomqvist, B. Johansson, O. Srivastava, R. Ahuja, *Excellent Catalytic Effects of Graphene Nanofibers on Hydrogen Release of Sodium Alanate*, **J. Phys. Chem. C** **116**, 10861 (2012).

55. J. Nisar, C. Moyses Araujo, R. Ahuja, *Water Interaction with native defects on rutile TiO₂ nanowire: Ab initio calculations*, **Appl. Phys. Lett.** **98**, 083115 (2011).

54. R. H. Scheicher, Sa Li, C. Moyses Araujo, A. Blomqvist, R. Ahuja, and P. Jena, *Theoretical study of C₆₀ as catalyst for dehydrogenation of LiBH₄*, **Nanotechnology** **22**, 335401 (2011).
53. C. Århammar, A. Pietzsch, N. Bock, E. Holmstrom, C. Moyses Araujo, S. Zhao, S. Green, T. Peery, F. Hennies, S. Amerioun, A. Fohlisch, T. Schmitt, V. N. Strocov, G. A. Niklasson, D. C. Wallace, Jan -Erik Rubensson, B. Johansson, and R. Ahuja, *Unveiling the complex electronic structure of amorphous metal oxides*, **Proceedings of the National Academy of Sciences of USA (PNAS)** **108**, 6355 (2011).
52. P. Srepusharawoot, A. Blomqvist, C. Moyses Araujo, R. H. Scheicher, and R. Ahuja, Alkaline decorated in Zn-, Mg- and Ca- Iso-reticular Metal Organic Frameworks -16: a DFT study, **Int. J. Hyd. Energy** **36**, 555 (2011).
51. T. Hussain, B. Pathak, M. T. Adit, C. Moyses Araujo, R. Ahuja, *Ab initio study of lithium-doped graphane for hydrogen storage*, **Europhys. Lett.** **96**, 27013 (2011).
50. C. Moyses Araujo, M. Kapilashrami, X. Jun, O. D. Jayakumar, S. Nagar, Y. Wu, C. Århammar, B. Johansson, L. Belova, R. Ahuja, and K.V. Rao, Room temperature ferromagnetism in pristine MgO thin films, **Appl. Phys. Lett.** **96**, 232505 (2010).
49. A. Blomqvist, C. Moyses Araujo, R. H. Scheicher, P. Srepusharawoot, W. Li, P. Chen, R. Ahuja, *Hydrogen as Promoter and Inhibitor of Superionicity: a Case Study on Li-N-H Systems*, **Phys. Rev. B.** **82**, 024304 (2010).
48. A. Blomqvist, G. Palsson, C. Moyses Araujo, R. Ahuja and B. Hjörvarsson, *Significance of self-trapping on hydrogen diffusion*, **Phys. Rev. Lett.** **105**, 185901 (2010).
47. C. Århammar, C. Moyses Araujo, K. V. Rao, S Norgren, B. Johansson and R. Ahuja, *First-principles investigation of magnetic properties of V-doped MgO: bulk and (001) surface*, **Phys. Rev. B** **82**, 134406 (2010).
46. W. Li, G. Wu, C. Moyses Araujo, R. H. Scheicher, A. Blomqvist, R. Ahuja, Z. Xiong, Y. Feng and P. Chen, *Li⁺ Ion Conductivity and Diffusion Mechanism in α -Li₃N and β -Li₃N*, **Energy & Environmental Science** **3**, 1524 (2010).
*I am the first-author from the theory team.
45. L. Huang, Cecilia Århammar, C. Moyses Araujo, F. Silvearv, and R. Ahuja, *Tuning magnetic properties of In₂O₃ by control of intrinsic defects*, **Europhys. Lett.** **89**, 47005 (2010).
44. L. Huang, F. Silvearv, C. Moyses Araujo, and R. Ahuja, *Defect induced strong ferromagnetism in Cr-doped In₂O₃ from first principles theory*, **Solid State Communication** **150**, 663-665 (2010).
43. Sa Li, R. Ahuja, C. Moyses Araujo, Börje Johansson, Puru Jena, *Dehydrogenation associated with Ti catalyst in sodium alanate*, **Journal of Physics and Chemistry of Solids** **71**, 1073-1076 (2010).

42. J. Nisar, C. Moyses Araujo, and R. Ahuja, *Structural, electronic and energetic properties of water adsorbed on β -Si₃N₄ (0001) surface: First-principles calculations*, **Surface Science** **604**, 616–621 (2010).
41. P. Srepusharawoot, A. Blomqvist, C. Moyses Araujo, R. H. Scheicher, and R. Ahuja, *One-dimensional polymeric carbon structure based on five-membered rings in alkaline earth metal dicarbides BeC₂ and MgC₂*, **Phys. Rev. B** **82**, 125439 (2010).
40. Wen Li, Ralph H. Scheicher, C. Moyses Araujo, Andreas Blomqvist, Rajeev Ahuja, and Ping Chen, *Understanding from First Principles why LiNH₂BH₃•NH₃BH₃ shows Improved Dehydrogenation over LiNH₂BH₃ and NH₃BH₃*, **J. Phys. Chem. C** **114**, 19089 (2010).
39. C. Århammar, C. Moyses Araujo and R. Ahuja, *Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia: First-principles calculations*, **Phys. Rev. B** **80**, 115208 (2009).
38. J. Wang, T. Liu, G. Wu, Y. Liu, C. Moyses Araujo, R. H. Scheicher, R. Ahuja, Z. Xiong, P. Yang, M. Gao, H. Pan, and P. Chen, *Potassium Modified Mg(NH₂)₂-2LiH System for Hydrogen Storage*, **Angewandte Chemie International Edition** **48**, 5828 (2009).
37. C. Moyses Araujo, A. Blomqvist, R. H. Scheicher, and R. Ahuja, *Superionicity in the Hydrogen Storage Material Li₂NH: Molecular Dynamics Simulations*, **Phys. Rev. B** **79**, 172101 (2009).
36. P. A. Berseth, A. G. Harter, R. Zidan, A. Blomqvist, C. Moyses Araujo, R. H. Scheicher, R. Ahuja, and P. Jena, *Carbon Nanomaterials as Catalysts for Hydrogen Uptake and Release in NaAlH₄*, **Nano Letters** **9**, 1501-1505 (2009).
35. L. Huang, C. Moyses Araujo, and R. Ahuja, *Magnetic and electronic properties of 3d transition-metal-doped In₂O₃: An ab-initio study*, **Europhys. Lett.** **87**, 27013 (2009).
34. P. Srepusharawoot, Ralph H. Scheicher, C. Moyses Araujo, Andreas Blomqvist, and R. Ahuja, *Ab Initio Study of Hydrogen Adsorption in Covalent Organic Framework-1*, **J. Phys. Chem. C** **113**, 8498 (2009).
33. P. Srepusharawoot, C. Moyses Araujo, A. Blomqvist, R. H. Scheicher and R. Ahuja, *A comparative investigation of H₂ adsorption strength in Cd- and Zn-based Metal Organic Framework-5*, **J. Chem. Phys.** **129**, 164104 (2008).
32. P. Larsson, C. Moyses Araujo, J. A. Larsson, P. Jena and R. Ahuja, *Role of catalysts in dehydrogenation of MgH₂ nanoclusters*, **Proceedings of the National Academy of Sciences of USA (PNAS)** **105**, 8227 (2008).

*I have contributed as much as the first author.

31. C. Moyses Araujo, A. Blomqvist and R. Ahuja, *Ti-induced destabilization of NaBH_4 from first-principles theory*, **J. Phys.: Cond. Matter – Fast track communication - 20**, 122202 (2008).
30. C. Moyses Araujo, Ralph H. Scheicher, and R. Ahuja, *Thermodynamic analysis of hydrogen sorption reactions in Li-Mg-N-H systems*, **App. Phys. Lett.** **92**, 021907 (2008).
29. D. Y. Kim, S. Lebegue, C. Moyses Araujo, B. Arnaud, M. Alouani and R. Ahuja, *Structurally induced insulator-metal transition in solid oxygen: A quasiparticle investigation*, **Phys. Rev. B** **77**, 092104 (2008).
28. A. Blomqvist, C. Moyses Araujo, P. Srepusharawoot, and R. Ahuja, *Li-decorated metal-organic framework 5: A route to achieving a suitable hydrogen storage medium*, **Proceedings of the National Academy of Sciences of USA (PNAS)** **104**, 20173 (2007).
* I have contributed as much as the first author.
27. C. Moyses Araujo, R. H. Scheicher, P. Jena and R. Ahuja, *On the structural and energetic properties of the hydrogen absorber $\text{Li}_2\text{Mg}(\text{NH})_2$* , **Appl. Phys. Lett.** **91**, 091924 (2007).
26. A Blomqvist, C. Moyses Araujo, P. Jena and R. Ahuja, *Dehydrogenation from 3d-transition metal doped NaAlH_4 : Prediction of New Catalysts*, **Appl. Phys. Lett.** **90**, 141904 (2007).
25. S. Lebegue, C. Moyses Araujo, O. Eriksson, B. Arnaud, M. Alouani, and R. Ahuja, *Quasiparticle and optical properties of BeH_2* , **Journal of Physics: Condensed Matter** **19**, 036223 (2007).
24. C. Moyses Araujo, S. Li, R. Ahuja, and P. Jena, *Vacancy mediated hydrogen desorption in sodium alanate*, **Phys. Rev. B** **72**, 165101 (2005).
23. C. Moyses Araujo, R. Ahuja, P. Jena, and J. M. Osorio Guillén, *Role of Titanium in hydrogen desorption in crystalline sodium-alanate*, **Appl. Phys. Lett.** **86**, 251913 (2005).
22. C. Moyses Araujo, R. Ahuja, A. V. Talyzin, and B. Sundqvist, *Pressure-induced phase transition in NaBH_4* , **Phys. Rev. B** **72**, 054125 (2005).
21. C. Moyses Araujo, S. Lebegue, O. Eriksson, B. Arnaud, M. Alouani, and R. Ahuja, *Electronic and optical properties of α , γ and β phases of MgH_2 : A first-principle GW investigation*, **J. of Appl. Phys.** **98**, 096106 (2005).
20. A Ferreira da Silva, I. Pepe, C. Persson, J. S. de Almeida, C. Moyses Araujo, R. Ahuja, B. Johansson, C. Y. An, and J.-H. Guo, *Optical Properties of Oxide Compounds PbO , SnO_2 and TiO_2* , **Physica Scripta** **T109**, 180 (2004).

19. R. Ahuja, C. Persson, A. Ferreira da Silva, J. Souza de Almeida, C. Moyses Araujo, B. Johansson, *Optical properties of SiGe Alloys*, **Journal of Applied Physics** **93**, 3832 (2003).

18. R. Ahuja, R. Arwin, A. Ferreira da Silva, C. Persson, J. M. Osorio-Guillen, J. Souza de Almeida, C. Moyses Araujo, E. Veje, N. Veissid, C. Y. An, I. Pepe and B. Johansson, *Electronic and Optical Properties of Lead Iodide*, **Journal of Applied Physics** **92**, 7219 (2002).

17. C. Moyses Araujo, A. Ferreira da Silva and Erasmo A. de Andrada e Silva, *Electron spin-orbit split minibands in semiconductor asymmetric superlattices*, **Phys. Rev. B** **65**, 235305 (2002).

* Selected for the June-2002 issue of the virtual journal of Nanoscale Science and Technology.

16. C. Persson, Bo E. Sernelius, A. Ferreira da Silva, C. Moyses Araujo, R. Ahuja, and B. Johansson, *Optical and reduced band gap in n- and p-type GaN and AlN*, **Journal of Applied Physics** **92**, 3207 (2002).

15. J. Souza de Almeida, C. Moyses Araujo, I. Pepe, A. Ferreira da Silva, Electrical field effects in two-dimensional disordered Hubbard-Mott model, **Phys. Rev. B** **66**, 035327 (2002).

14. L. A. Silva, J. B. Andrade, C. Moyses Araujo, O. Nakamura, A. Ferreira da Silva, M. S. O. Massunaga and H. Vargas, *Characterization of the double sulfites $Cu_2SO_3 \cdot MSO_3 \cdot 2H_2O$ ($M = Cu, Fe, Mn$ or Cd) by photothermal techniques*, **Phys. Chem. Chem. Phys.** **3**, 4800 (2001).

13. C. Moyses Araujo, Jailton Souza de Almeida, I. Pepe, A. Ferreira da Silva, Bo E. Sernelius, J. Pereira de Souza and H. Boudinov, *Band-gap shift of the heavily single and doubly-donor systems Si:Bi and Si:P,Bi*, **Phys. Rev. B** **62**, 12882 (2000).

Peer-reviewed conference contributions

12. C. Moyses Araujo, and R. Ahuja, *Electronic and optical properties of pressure induced phases of MgH_2* , **Journal of Alloys and Compounds** **404**, 220 (2005).
Proceedings of the 9th International Symposium on Metal-Hydrogen Systems, Fundamentals and Applications (MH2004), Cracow, Poland, 2004.

11. M. Emilsson, C. Moyses Araujo and R. Ahuja, *Hydrogen Desorption in High Pressure Phases of MgH_2 : A Density Functional Theory Based Study*, **Proceedings of Second International Symposium on Hydrogen in Matter**, edited by B. Hjörvarsson and G. R. Myneni, AIP Conference Proceedings 837, ISBN 0-7354-0329-5, 2005.

10. C. Moyses Araujo, A. Ferreira da Silva and R. Ahuja, Pressure induced phase transition in ErH_3 , **physica status solidi (b)** **241**, 3219 (2004).
Proceedings of the 11th International Conference on High-Pressure Semiconductor Physics (HPSP-11), Berkeley, USA, 2-5 August 2004.
9. C. Moyses Araujo, A. Ferreira da Silva, C. Persson, R Ahuja and E. A. de Andrada e Silva, *Spin-dependent conductance in nonmagnetic InGaAs asymmetric double barrier device*, **Brazilian Journal of Physics** **34**, 632 (2004).
8. C. Moyses Araujo, A. Ferreira da Silva, E. A. de Andrada e Silva, *Transmission through spin-split conduction minibands in nonmagnetic semiconductor superlattices*, **Proceedings of the 26th International Conference on the Physics of Semiconductors**, edited by A. R. Long and J. H. Davies (Bristol (UK) and Philadelphia (USA)), 2003.
7. C. Moyses Araujo, A. Ferreira da Silva and E. A. de Andrada e Silva, *Resonant tunneling of polarized electrons through nonmagnetic III-V semiconductor multiple barriers*, **Brazilian Journal of Physics** **32**, 321 (2002).
Proceedings of the 10th Brazillian Workshop on Semiconductor Physics (BWSP 10), Guarujá, Brazil, 22-27 April, 2001.
6. C. Moyses Araujo, J. R. L. Fernandez, A. Ferreira da Silva, I. Pepe, J. R. Leite, Bo E. Sernelius, A. Tabata, C. Persson, R. Ahuja, D. J. As, D. Schikora, and K. Lischka, *Electrical resistivity, MNM transition and band-gap narrowing of cubic GaN:Si*, **Microelectronics Journal** **33**, 365 (2002).
Proceedings of the 1st Ibero-American Workshop on Semiconductor Nanostructures: Micro and Optoelectronics Applications, Mexico City, Mexico, 20-24 November, 2000.
5. A. Ferreira da Silva, C. Moyses Araujo, Bo E. Sernelius, C. Persson, R Ahuja and B. Johansson, *Influence of Si doping on optical properties of wurtzite GaN*, **J. Phys.: Condens. Matter** **13**, 8891 (2001).
Proceedings of the Conference on Doping Issues in Wide Band-Gap Semiconductors, Univ. Exeter, Exeter, England, 21-23 March, 2001.
4. J. Souza de Almeida, C. Moyses Araujo, I. Pepe and A. Ferreira da Silva, *Electrical field effects in n-type MOSFET and metal-nonmetal transition*, **Microelectronics Journal** **33**, 371 (2002).
Proceedings of the 1st Ibero-American Workshop on Semiconductor Nanostructures: Micro and Optoelectronics Applications, Mexico City, Mexico, 20-24 November, 2000.
3. J. R. L. Fernandez, C. Moyses Araujo, A. Ferreira da Silva, J.R. Leite, Bo E. Sernelius, A. Tabata, E. Abramof, V. A. Chitta, C. Persson, R. Ahuja, I. Pepe, D. J. As, T. Frey, D. Schikora, K. Lischka, *Electrical resistivity and band-gap shift of Si-doped GaN and metal-nonmetal transition in cubic GaN, InN and AlN systems*, **Journal of Crystal Growth** **231**, 420 (2001).

Proceedings of the International Specialist Meeting on Bulk Nitride Growth and Related Techniques, Foz do Iguacu, Brazil, 12-16 November, 2000.

Book chapters and books

2. C. Moyses Araujo and R. Ahuja

Electronic Structure and High-Pressure Behavior of Solids.

Book Chapter in Thermodynamics Properties of Solids: Experiment and Modeling, eds. S. L. Chaplot, R. Mittal, and N. Choudhury (WILEY-VCH, Weinheim) – 2010.

1. C. Moyses Araujo

Hydrogen Storage Materials: Design, Catalysis, Thermodynamics, Structure and Optics

PhD Thesis, Uppsala University, ISBN 978-91-554-7129-3, 2008.

Website: <http://publications.uu.se/theses/abstract.xsql?dbid=8574>.

***This Thesis has been selected for a press release by Uppsala University:**

<http://www.uu.se/en/news/news-document/?id=351&area>

IX. Organisation of Scientific Meetings

2015 – Co-Chairman of the workshop *Promising Approaches for Conversion and Storage of Solar Energy*, October 8-9 2015, Medellin, Colombia.

2013 – Co-chairman of the symposium *Hydrogen Storage, Production & Fuel Cell* in SMEC meeting, March 23-30 2013, Miami, USA.

2010 – Organizing committee member, *48th European High Pressure Research Group Conference (EHPRG)*, 25-29 July 2010 – Uppsala, Sweden.

2007 – Organizing committee member, *Swedish-Brazilian Workshop on Advanced Functional Materials*, Salvador, Brazil.

X. Attendance in workshops, conferences and symposiums (with work presentations)

2013 – Nordic Battery Conference, Uppsala University, **Uppsala, Sweden.**

2013 – ISACS12 Challenges in Chemical Renewable Energy, **Cambridge, UK.**

2012 – *CECAM Conference: "Energy from the Sun: Computational Chemists and Physicists Take up the Challenge"* **Cagliari, Italy.**

2012 – *244th ACS National Meeting 2012, [Energy & Fuels Division](#), Philadelphia, PA, USA.*

2011 – *Workshop on Computational Chemistry*, GE global research center, **NY, USA.**

2010 – *Psi_k Conference*, **Berlin, Germany.**

2009 – *MRS Fall Meeting*, **Boston, MA, USA.**

2009 – *6th meeting of the Nordic Network of Excellence on Hydrogen Storage Materials*, **Vilnius, Lithuania.**

2008 – *MRS Fall Meeting*, **Boston, MA, USA.**

2008 – *BAHIATEC – International Symposium of Innovation*, **Brazil.**

2008 – 4th meeting of the Nordic Network of Excellence on Hydrogen Storage Materials, **Copenhagen, Denmark.**

2008 – *International Symposium on Metal-Hydrogen systems*, **Reykjavik, Iceland.**

2007 – *Gordon Research Conferences: Hydrogen-Metal Systems*, **Colby College in Waterville, ME, USA.**

2007 – *International Symposium on Hydrogen Storage*, **Miami Beach, USA.**

2006 – *International Symposium on Metal-Hydrogen Systems*, **Lahaina, Maui, Hawaii, USA.**

2005 – *Workshop on Hydrogen Storage with Novel Nanomaterials*, **Bad Honnef, Germany.**

2005 – *Second International Symposium on Hydrogen in Matter*, **Uppsala Sweden.**

2004 – *International symposium on metal-hydrogen systems, fundamentals&applications*, **Cracow, Poland.**

2004 – *Eleventh International Conference on High Pressure Semiconductor Physics*, **Berkeley, California, USA.**

2004 – *Third network meeting of “EXCITING”*: Mid-term evaluation meeting, **Aarhus, Denmark.**

2003 – *Research Training Network on Computational Magnetolectronics*: Annual Meeting, **Halle, Germany.**

2003 – *Workshop on Dynamics in Magnetic Materials*, **Uppsala University, Sweden.**

2003 – *Light Metals for Hydrogen Storage*, **Uppsala University, Sweden.**

XI. Commissions of Trust

2015 – Academic coordinator of the Swedish Academic Collaboration Forum for the organization of excellence seminar in Brazil in May 16-18, 2016.

2014 – present: Committee member for the development of a novel international master program between Uppsala University and University of Sao Paulo in Brazil.

2013 – Member of Uppsala University’s delegation to promote Swedish education in the STINT Excellence Seminar in Brazil.

2012 – Member of the evaluation committee for the Master thesis at Federal University of Bahia, Salvador, Ba, Brazil.

2011 – Member of the evaluation committee for the Master thesis at Federal University of Bahia, Salvador, Ba, Brazil.

2010 – Guest-editor of the International Journal of High Pressure Research for the proceedings of the 48th European High Pressure Research Group Conference (EHPRG).

2010 – Member of the evaluation committee for the PhD thesis at Royal Institute of Technology (KTH), Stockholm, Sweden.

- Reviewer for >8 international scientific journals.