

Curriculum Vitae

Egill Skúlason

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Date of Birth 10th of March 1979
Citizenship Icelandic
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Education

- **Ph.D., *Engineering Physics*, Oct 2009.**
Center for Atomic-scale Materials Design (CAMd)
Technical University of Denmark (DTU)
Thesis Advisors: Professor Jens K. Nørskov
(now Professor of Chemical Engineering, Stanford University)
- **M.Sc. *Computational Chemistry*, June 2005.**
Department of Chemistry, University of Iceland
Thesis Advisors: Professor Hannes Jónsson
- **B.Sc. *Chemistry*, June 2003,** Department of Chemistry, University of Iceland
- **B.Sc. *Biochemistry*, June 2003,** Department of Chemistry, University of Iceland

Professional Career

- *Professor of Chemical Engineering*, School of Engineering and Natural Sciences, Department of Industrial Engineering, Mechanical Engineering and Computer Science, U. Iceland, **July 2018 – present**
- *Chief Scientific Officer and Chairman of the Board*, Atmonia (spin-off company), **Nov 2016 – present**
- *Visiting Professor at DTU Energy*, Technical University of Denmark, **April 2018 – June 2018**
- *Professor of Chemistry*, School of Engineering and Natural Sciences, Department of Physical Sciences, U. Iceland, **July 2016 – June 2018**
- *Associate Professor*, School of Engineering and Natural Sciences, Physical Sciences, Department of Chemistry, U. Iceland, **July 2014 – June 2016**
- *Assistant Professor*, School of Engineering and Natural Sciences, Physical Sciences, Department of Chemistry and Department of Physics, U. Iceland, **Nov 2013 – June 2014**
- *Titled Engineer*, Ministry of Industry and Innovation, Iceland, **May 2012**
- *Research Assistant Professor*, Science Institute, Chemistry Division, U. Iceland, **Oct 2010 – Oct 2013**
- *Adjunct*, Department of Chemistry, U. Iceland, **June 2011 – Oct 2013**
- *Post-doc*, Science Institute, Chemistry Division, U. Iceland, **Aug 2009 – Sep 2010**
- *Research Fellow*, CAMd, DTU, **Sep 2005 – July 2009.**
- *Research Fellow*, Department of Chemistry, U. Iceland, **June 2003 – Aug 2005.**

- B.S. research project (funded by The Student Innovation Fund), *Light and Seasonally Affected Disorder*, U. Iceland, **summer 2002**.
- *Research Project*, Research lab, Alcan in Iceland, **summer 2001**.
- *Chemical Analysis*, Research lab, Alcan in Iceland, **summer 2000**.

Awards

- Icelandic Science and Technology Policy Council “Young Scientist Encouragement Award”, **Nov 2015**
- The University of Iceland Applied Science Prize for the project “Catalyst Engineering: Economical Fertilizer Production”, **Nov 2013**

Administration

- Panel member of the University of Iceland Research Fund, **Sept 2017 - present**
- Chairman and panel member of the Icelandic Research Fund expert panel for Physical Sciences and Mathematics, **Sept 2015 – March 2017 & June 2019 - present**
- Establishing and maintaining programs in *Chemical Engineering* and *Engineering Physics* at the School of Engineering and Natural Sciences at the University of Iceland, **Sept 2013 – present**

Research Funding (Principal Investigator)

- *The Doctoral Fund of the University of Iceland*, “Direct electrochemical nitrogen oxidation to nitrate using transition metal oxide catalysts”, (1 Ph.D. student) **2019-2022**
- *The Icelandic Research Fund*, Grant of Excellence: “Artificial nitrogen fixation at ambient conditions through rational catalyst design”, 3 Ph.D. students and 2 Postdoctoral fellows, (150 million ISK or ~1.25 million USD) **2019-2021**
- *The Icelandic Technology Development Fund*, “Catalyst optimization for sustainable ammonia”, (10 million ISK or 100 thousand USD) **2017-2018**
- *The Icelandic Technology Development Fund*, “Fertilizer from air and water: Towards application”, (41 million ISK or 400 thousand USD) **2017-2020**
- *The Doctoral Fund of the University of Iceland*, “Designing catalysts for sustainable fuel production”, (1 Ph.D. student) **2018-2020**
- *The Icelandic Research Fund*, Grant of Excellence: “Fertilizer from air and water: From theory to experiments”, several Ph.D. students and several Postdoctoral fellows, (125 million ISK or ~1.2 million USD) **2015-2017**
- *The Icelandic Research Fund*, Project grant: “Electrochemical production of fertilizer and green fuel”, 1 Ph.D. student and 1 Postdoctoral fellow, (20 million ISK) **2012-2014**
- *The Icelandic Research Fund*, Postdoctoral grant: “Electrochemical fixation of CO₂”, (13.5 million ISK) **2010-2012**
- *The Research Fund of University of Iceland*, “Defects in external electric field”, (500 thousands ISK) **2011**, (1300 thousands ISK) **2012**, “Designing catalysts for fuel cells and solar cells”, (800 thousands ISK) **2013**, (1100 thousands ISK) **2014**, (700 thousands ISK) **2015**, (700 thousands ISK) **2016**, (1100 thousands ISK) **2017**, (700 thousands ISK) **2018**
- *The Student Innovation Fund*, “CO₂ electroreduction to fuel using copper nanoparticles”, 3 students, (2097 thousands ISK), **summer 2017**
- *The Student Innovation Fund*, “CO₂ to green fuel”, 3 students, (2097 thousands ISK), **summer 2016**

- *The Student Innovation Fund*, “From emissions to fuel”, 3 students, (2097 thousands ISK), **summer 2015**
- *The Student Innovation Fund*, “Catalyst design for future fuel production”, 3 students, (1020 thousands ISK), **summer 2014**
- *The Student Innovation Fund*, “Producing fuel from sunlight, water and CO₂”, 3 students, (1020 thousands ISK), **summer 2013**
- *The Student Innovation Fund*, “Electrochemical production of fertilizer from atmospheric nitrogen”, 3 students, (1020 thousands ISK), **summer 2012**
- *The Student Innovation Fund*, “Simulation of hydrogen diffusion in external electric field”, 1 student, (340 thousands ISK), **summer 2011**
- *The Student Innovation Fund*, “Mechanism of N₂ fixation on nano-structures”, 2 students, (560 thousands ISK), **summer 2010**

Regular Reviewer for Journals:

- Nature Energy, Nature Catalysis, Nature Communications etc.
- ACS Sustainable Chemistry and Engineering, ACS Catalysis etc.
- Catalysis Letters, Journal of Catalysis, Topics in Catalysis, Catalysis Today
- ChemCatChem, ChemSusChem
- Journal of Physical Chemistry
- Surface Science, Applied Surface Science
- European Physical Journal B, Physica B
- Journal of Molecular Catalysis, Journal of Alloys and Compounds
- Journal of the American Chemical Society
- Joule

Teaching Experience

- Current topics in Chemistry and Biochemistry (seminar chair), UI, **2015, 2016, 2017**
- *General Chemistry 1*, UI, **2014, 2015, 2016, 2017, 2018, 2019**
- *Chemistry 1*, UI, **2012, 2013**.
- *Applying Mathematics and Physics in Chemistry*, UI, **2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017**
- *Computations in Chemistry*, UI, **2009, 2010, 2011, 2012, 2013, 2014**
- *Physical Chemistry A*, (a few lectures) UI, **2011**.
- *Thermodynamics and Introduction to Statistical Mechanics*, (a few lectures) UI, **2009, 2011, 2012**.
- *Advanced quantum mechanics*, (one lecture) DTU, **2008**
- *Organic Chemistry 1*, (Laboratory Teacher), UI, **2004**.
- *General Chemistry 1*, (Laboratory Teacher), UI, **2003**.

Student Advising Experience

- *Advising* 5 Post-docs, 5 Ph.D., 1 M.Sc., 1 research assistant and 25 B.Sc. students
- *Co-advising* 3 Ph.D, 3 M.Sc. and 4 B.Sc. students

Career breaks

March 2008 – Nov 2008 (8 months) Paternity leave
 Sept 2013 – Nov 2013 (2 months) Paternity leave

Publications (ISI journals)

Google scholar: Citations: 4049, h-index: 24

ISI: Citations: 3196, h-index: 22

36. "Elucidating the mechanism of electrochemical N₂ reduction at the Ru (0001) electrode"
E. Tayyebi, Y. Abghoui, E. Skúlason
ACS Catalysis, **In Press** (2019)
35. "Biomimetic nitrogen fixation catalyzed by transition metal sulfide surfaces in an electrolytic cell"
Y. Abghoui, S.B. Sigtryggsson, E. Skúlason
ChemSusChem, **12** (2019) 4265
34. "Catalytic trends of nitrogen doped carbon nanotubes for oxygen reduction reaction"
M. Van den Bossche, E. Skúlason, C. Rose-Petruck & H. Jónsson
Nanoscale, **11** (2019) 18683
33. "Elucidation of temperature-programmed desorption of high-coverage hydrogen on Pt (211), Pt (221), Pt (533) and Pt (553) based on density functional theory calculations"
M.J. Kolb, A.L. Garden, C. Badan, J.A.G. Torres, E. Skúlason, L.B.F. Juurlink, H. Jónsson & M.T.M. Koper
Physical Chemistry Chemical Physics, **21** (2019) 17142
32. "Assessment of constant-potential implicit solvation calculations of electrochemical energy barriers for H₂ evolution on Pt"
M. Van den Bossche, E. Skúlason, C. Rose-Petruck & H. Jónsson
Journal of Physical Chemistry C, **123** (2019) 4116
31. "Calculations of product selectivity in electrochemical CO₂ reduction"
J. Hussain, H. Jónsson & E. Skúlason
ACS Catalysis, **8** (2018) 5240
30. "Trends of electrochemical CO₂ reduction reaction on transition metal oxide catalysts"
E. Tayyebi, J. Hussain, Y. Abghoui & E. Skúlason
Journal of Physical Chemistry C, **122** (2018) 10078
29. "Hydrogen evolution reaction catalyzed by transition metal nitrides"
Y. Abghoui & E. Skúlason
Journal of Physical Chemistry C, **121** (2017) 24036
28. "Computational screening of rutile oxides for electrochemical ammonia formation"
Á.B. Höskuldsson, Y. Abghoui, A.B. Gunnarsdóttir & E. Skúlason
ACS Sustainable Chemistry & Engineering, **5** (2017) 10327
27. "Atomic scale simulations of heterogeneous electrocatalysis: recent advances"
E. Skúlason & H. Jónsson
Advances in Physics: X, **2** (2017) 481

26. "Computational Predictions of Catalytic Activity of Zincblende (110) Surfaces of Metal Nitrides for Electrochemical Ammonia Synthesis"
Y. Abghoui & E. Skúlason
Journal of Physical Chemistry C, **121** (2017) 6141
25. "Electrochemical synthesis of ammonia via Mars-van Krevelen mechanism on the (111) facets of group III–VII transition metal mononitrides"
Y. Abghoui & E. Skúlason
Catalysis Today, **286** (2017) 78
24. "Onset potentials for different reaction mechanisms of nitrogen activation to ammonia on transition metal nitride electro-catalysts"
Y. Abghoui & E. Skúlason
Catalysis Today, **286** (2017) 69
23. "Faraday efficiency and mechanism of electrochemical surface reactions: CO₂ reduction and H₂ formation on Pt(111)"
J. Hussain, H. Jónsson & E. Skúlason
Faraday Discuss. **195** (2016) 619
22. "Electroreduction of N₂ to ammonia at ambient conditions on mononitrides of Zr, Nb, Cr, and V – A DFT guide for experiments",
Y. Abghoui, A.L. Garden, J. Howalt, T. Vegge & E. Skúlason,
ACS Catalysis, **6** (2016) 635
21. "On the pH dependence of electrochemical proton transfer barriers"
J. Rossmesl, K. Chan, E. Skúlason, M. E. Björketun & V. Tripkovic,
Catalysis Today **262** (2016) 36
20. "The mechanism of industrial ammonia synthesis revisited: Calculations of the role of the associative mechanism",
A. L. Garden & E. Skúlason,
Journal of Physical Chemistry C **119** (2015) 26554.
19. "Enabling electrochemical reduction of nitrogen to ammonia at ambient conditions through rational catalyst design",
Y. Abghoui, A. L. Garden, S. Björgvinsdóttir, V.F. Hlynsson, H. Ólafsdóttir & E. Skúlason,
Physical Chemistry Chemical Physics **17**, (2015) 4909
18. "Stability and magnetism of transition metal nitride surfaces"
V. F. Hlynsson, E. Skúlason & A. L. Garden
J. Alloys and Compounds **604**, (2014) 172.
17. "Catalytic activity of Pt nano-particles in H₂ formation",
E. Skúlason, A. A. Faraj, L. Kristinsdóttir, J. Hussain, A.L. Garden & H. Jónsson,
Topics in Catalysis **57**, (2014) 273.
16. "Hydrogen adsorption and desorption at the Pt(110)-(1x2) surface: Experimental and theoretical study",
S. Gudmundsdóttir, E. Skúlason, K.-J. Weststrate, L. Juurlink & H. Jónsson,
Physical Chemistry Chemical Physics **15**, (2013) 6323.
15. "Modeling of the symmetry factor of electrochemical proton discharge via

- the Volmer reaction",
M. E. Björketun, V. Tripkovic, E. Skúlason & J. Rossmeisl,
Catalysis Today, **202** (2013) 168.
14. "Local density of states analysis using Bader decomposition for N₂ and CO₂ adsorbed on Pt(110)-(1x2) electrodes",
S. Gudmundsdóttir, W. Tang, G. Henkelman, H. Jónsson & E. Skúlason,
Journal of Chemical Physics, **137**, (2012) 164705.
 13. "A systematic DFT study of hydrogen diffusion on transition metal surfaces",
L. Kristinsdóttir, and E. Skúlason,
Surface Science, **606** (2012) 1400.
 12. "Reentrant mechanism for associative desorption: H₂/Pt(110)-(1x2)",
S. Gudmundsdóttir, E. Skúlason & H. Jónsson,
Physical Review Letters, **108** (2012) 156101
 11. "A theoretical evaluation of possible transition metal electro-catalyst for N₂ reduction",
E. Skúlason, T. Bligaard, S. Gudmundsdóttir, F. Studt, J. Rossmeisl, F. Abild-Pedersen, T. Vegge, H. Jónsson & J.K. Nørskov,
Physical Chemistry Chemical Physics, **14** (2012) 1235
 10. "Universal transition state scaling relations for hydrogenation and dehydrogenation reactions over transition metals"
S. Wang, V. Petzold, V. Tripkovic, J. Kleis, J. G. Howalt, E. Skúlason, E. M. Fernández, B. Hvolbæk, G. Jones, A. Toftelund, H. Falsig, M. Björketun, F. Studt, F. Abild-Pedersen, J. Rossmeisl, J. K. Nørskov & T. Bligaard,
Physical Chemistry Chemical Physics, **13** (2011) 20760.
 9. "The standard hydrogen electrode and potential of zero charge in density functional calculations"
V. Tripkovic, M. E. Björketun, E. Skúlason & J. Rossmeisl,
Physical Review B, **84** (2011) 115452.
 8. "Modeling the electrochemical hydrogen oxidation and evolution reactions on the basis of density functional theory calculations",
E. Skúlason, V. Tripkovic, M. Björketun, S. Gudmundsdóttir, G.S. Karlberg, J. Rossmeisl, T. Bligaard, H. Jónsson & J.K. Nørskov,
Journal of Physical Chemistry C **114** (2010) 18182.
 7. "The oxygen reduction reaction mechanism on Pt(111) from density functional theory calculations",
V. Tripkovic, E. Skúlason, S. Siahrostami, J.K. Nørskov & J. Rossmeisl,
Electrochimica Acta, **55** (2010) 7975
 6. "Hydrogen adsorption on palladium and palladium hydride at 1 bar"
M. Johansson, E. Skúlason, G. Nielsen, S. Murphy, R. Nielsen & I. Chorkendorff,
Surface Science **604** (2010) 718
 5. "Modeling the electrified solid-liquid interface"
J. Rossmeisl, E. Skúlason, M.E. Björketun, V. Tripkovic & J.K. Nørskov
Chemical Physics Letters **466** (2008) 68

4. "Cyclic voltammograms for H on Pt(111) and Pt(100) from first principles"
G.S. Karlberg, T.F. Jaramillo, E. Skúlason, J. Rossmeisl, T. Bligaard & J.K.Nørskov,
Physical Review Letters, **99** (2007) 126101
3. "Scaling properties of adsorption energies for hydrogen containing molecules on transition metal surfaces"
F. Abild-Pedersen, J. Greeley, F. Studt, J. Rossmeisl, T.R. Munter, P.G.Moses, E. Skúlason, T.Bligaard & J.K.Nørskov,
Physical Review Letters, **99** (2007) 016105
2. "Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode"
E. Skúlason, G. S. Karlberg, J. Rossmeisl, T. Bligaard, J. Greeley, H. Jónsson & J. K. Nørskov,
Physical Chemistry Chemical Physics, **9** (2007) 3241
1. "Predicting catalysis: Understanding ammonia synthesis from first-principles calculations"
A. Hellman, M. Biczysko, T. Bligaard, C. H. Christensen, D. C. Clary, S. Dahl, R. van Harreveld, K. Honkala, H. Jónsson, M. Luppi, E. J. Baerends, G. J. Kroes, U. Manthe, J. K. Nørskov, R. A. Olsen, J. Rossmeisl, E. Skúlason, C. S. Tautermann, A. J. C. Varandas & J. K. Vincent,
Journal of Physical Chemistry B, **110** (2006) 17719

Book chapter

A.L. Garden, Y. Abghoui and E. Skúlason, "Applications of metal nitrides as electrocatalysts", in "Novel Catalytic Materials", eds. J. Hargreaves, A. McFarlane, S. Laassiri, Royal Society of Chemistry, (2018)

Publications (Proceedings and Icelandic journal)

4. "Computational Study of Electrochemical CO₂ Reduction at Transition Metal Electrodes"
J. Hussain, E. Skúlason, H. Jónsson
Procedia Computer Science, **51** (2015) 1865
3. "Transition Metal Nitride Catalysts for Electrochemical Reduction of Nitrogen to Ammonia at Ambient Conditions"
Y. Abghoui, E. Skúlason
Procedia Computer Science, **51** (2015) 1897
2. "Modeling Electrochemical Reactions at the Solid-liquid Interface Using Density Functional Calculations"
E. Skúlason
Procedia Computer Science, **51** (2015) 1887
1. "Hvernig myndast vetnissameindin úr róteindum og rafeindum?"
E. Skúlason,
Raust – Tímarit um raunvísindi og stærðfræði **1** (2009) 73

Other Publications

- **Ph.D. Thesis:** *Modeling Electro-catalytic Reactions using Density Functional Theory Calculations*,
E. Skúlason, CAMd, DTU, Kongens Lyngby, Denmark, **Oct 2009**.
- **M.Sc. Thesis:** *Theoretical Calculations of Electrochemical Processes - Formation of Ammonia and Hydrogen*,
E. Skúlason, Department of Chemistry, U. Iceland, Reykjavik, Iceland, **June 2005**.
- **B.S. Research Thesis:** *Light and Seasonal Affective Disorder*,
E. Skúlason, The Student Innovation Fund, Reykjavik, Iceland, **Sep 2002**.

Organizer of Workshops and Summer Schools

- *CO₂ conversion to fuel*, NordCO₂ Autumn School, Uppsala, Sweden, **Oct 2019**.
- *Modeling methods in computational chemistry: theory and applications*,
Reykjavik, Iceland, **June 2016**.
- *Clusters 2014: Workshop on Reactivity and catalysis of metallic nano-clusters*,
Aalto University, Finland, **June 2014**.
- *Materials for the Hydrogen Society*, Reykjavik, Iceland, **June 2013**.

Opponent in Ph.D. defenses

- Ph.D. thesis by Nico Holmberg: *Hydrogen evolution reaction on carbon nanotubes: Insights from electronic structure theory*, School of Chemical Engineering, Aalto University, Finland, **May 2018**.
- Ph.D. thesis by Mateusz Reda: *Computational studies of non-precious catalysts for the oxygen reduction reaction*, Department of Energy Conversions and Storage, Technical University of Denmark, Denmark, **May 2018**.
- Ph.D. thesis by Arghya Bhowmik: *Design of oxide electrocatalysts for efficient conversion of CO₂ into liquid fuels*, Department of Physics, Technical University of Denmark, Denmark, **Aug 2017**.
- Ph.D. thesis by Manuel Kolb: *Water-Related Adsorbates on Stepped Platinum Surfaces*, Department of Chemistry, Leiden University, The Netherlands, **March 2016**.
- Ph.D. thesis by Rizwan Ahmed: *First Principle simulations of electrochemical interfaces - a DFT study*, Department of Physics, Technical University of Denmark, Denmark, **April 2015**.

Oral Presentations at Conferences

- *N₂ and CO₂ reduction reactions*, Workshop on: Computational Material Chemistry, Telluride, CO, USA, **July 2019**.
- *Electrochemical Nitrogen Reduction Reaction: From Theory to Experiments*, 26th North American Catalysis Society Meeting, Chicago, IL, USA, **June 2019**.
- *Calculations of product selectivity in CO₂ electroreduction*, International Bunsen-Discussion-Meeting, Taormina, Italy, **April 2019**.
- *Electrochemical reduction of CO₂ to fuel & N₂ to ammonia: DFT calculations & experiments*, 3rd Annual CADIAC meeting, Aarhus University, Aarhus, Denmark, **Nov 2018**.
- *Calculations of product selectivity in electrochemical CO₂ and N₂ reduction*, Computational Electrochemistry, Aalto University, Finland, **July 2018**.

- *Electrochemical CO₂ and N₂ reduction: low and high temperature electrolysis*, 4th International Workshop Prospects on Protonic Ceramic Cells, Bordeaux, France, **Oct 2017 (keynote)**.
- *New insight into the electrochemical CO₂ and N₂ reduction*, Fundamental electrocatalysis: Theory meets experiments, Lorentz Center, Leiden, The Netherlands, **June 2017**.
- *Electroreduction of CO₂ to hydrocarbons and alcohols*, 253rd American Chemical Society, San Francisco, California, USA, **April 2017**.
- *New insights into the electroreduction of CO₂ to hydrocarbons and alcohols*, 8th International Conference on Advanced Materials and Nanotechnology, Queenstown, New Zealand, **Feb 2017**.
- *Faraday efficiency and mechanism of electrochemical surface reactions: CO₂ reduction and H₂ formation on Pt(111)*, Royal Society of Chemistry: Faraday Discussions - Reaction Rate Theory, Cambridge, UK, **Sep 2016**.
- *Electrochemical reduction of CO₂ to hydrocarbons and alcohols and of N₂ to ammonia*, 4th Nordic meeting on organometallic chemistry, Reykjavik, Iceland, **March 2016**.
- *Mechanism of Electrochemical CO₂ Reduction to Methane on Metal Electrodes*, 24th North American Catalysis Society Meeting, Pittsburgh, PA, USA, **June 2015**.
- *Modeling electrochemical reactions at the solid-liquid interface using density functional calculations*, The International Conference on Computational Science, Workshop on Computational Chemistry and its Applications, Reykjavik University, Reykjavik, Iceland, **June 2015**.
- *CO₂ electro-reduction – Simulations of the solid/liquid interface*, Manufacturing green fuels from renewable energy, DTU Energy Conversion, Risø Campus, Denmark, **April 2015**.
- *Framleiðsla á áburði frá lofti og vatni*, VoN Rannsóknarþing, Reykjavik, Iceland, **Oct 2014**.
- *Is there a difference in catalytic activity between steps and edges on nanoparticles?*, Clusters 2014: Workshop on Reactivity and catalysis of metallic nano-clusters, Aalto University, Finland, **June 2014**.
- *New insights in dynamical processes from theoretical studies - Ways to move forward*, Elementary Reactive Processes at Surfaces, Lorentz center, Leiden, The Netherlands, **Dec 2012**.
- *Mechanism of hydrogen formation*, 22nd North American Catalysis Society Meeting, Detroit, MI, USA, **June 2011**.
- *Computer Simulations of the Electrified Solid-liquid Interface*, Applications and Methods of High Performance Computing, Reykjavik, Iceland, **April 2011**.
- *How do solvated protons and electrons combine to form H₂ molecules?*, Nano and Surface Science Approaches to Production and Storage of Hydrogen, Noordwijkerhout, The Netherlands, **Nov 2010**.
- *How do solvated protons and electrons combine to form H₂ molecules?*, VoN Rannsóknarþing, Reykjavik, Iceland, **Oct 2010**.
- *Simulations of atomic scale transitions at charged interfaces*, Ψ_k-2010 Conference, Berlin, Germany, **Sep 2010**.
- *Simulations of atomic scale transitions at charged interfaces*, Para 2010: State of the Art in Scientific and Parallel Computing, Reykjavik, Iceland, **June 2010**.
- *Towards Atomistic Understanding of Hydrogen Evolution*, Elementary Reactive Processes at Surfaces, San Sebastian, Spain, **Sep 2007**.

- *Molecular-level Picture of the Hydrogen Evolution*, Hydrogen EU-network meeting, Amsterdam, The Netherlands, **April 2007**.

Oral Presentations at Seminars

- *Rational electrocatalyst design towards a sustainable future*, Promotion Ceremony, School of Engineering and Natural Sciences, University of Iceland, Reykjavík, Iceland, **Des 2018**.
- *Electrochemical N_2 and CO_2 reduction: DFT calculations and experiments*, School of Chemical Engineering, Georgia Institute of Technology, Georgia, USA, **Sep 2018**.
- *Electrochemical CO_2 and N_2 reduction reactions*, Department of Chemistry, University of Copenhagen, Denmark, **May 2018**.
- *Calculations of product selectivity in electrochemical CO_2 reduction*, Kick-off meeting for NordCO₂, Tromsø, Norway **May 2018**.
- *Electro-catalytic CO_2 and N_2 reduction: From theory to experiments*, Department of Chemical Engineering, Stanford University, USA, **Jan 2018**.
- *Rational catalyst design for selective electroreduction of CO_2 to fuel and N_2 to ammonia*, Department of Chemical Engineering, University of California, Berkeley, USA, **Jan 2018**.
- *Electrochemical reduction of CO_2 and N_2 : DFT calculations and experiments*, Division of Chemistry and Chemical Engineering, California Institute of Technology, USA, **Jan 2018**.
- *New insights from theory and experiments into the electrochemical CO_2 and N_2 reduction*, Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, USA, **Jan 2018**.
- *Electroreduction of CO_2 and N_2 : Predictions from calculations and experimental validation*, Department of Chemistry, University of California, Santa Barbara, USA, **Jan 2018**.
- *New insights into the electroreduction of CO_2 to hydrocarbons and alcohols and of N_2 to ammonia*, Department of Chemical Physics, Stockholm University, Sweden, **March 2017**.
- *Electrochemical CO_2 and N_2 reduction: New insights from calculations*, Department of Chemistry, University of Otago, New Zealand, **March 2017**.
- *New insights into the electrochemical CO_2 and N_2 reduction*, MacDiarmid Institute for advance materials and nanotechnology and School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand, **Feb 2017**.
- *New insights into the electroreduction of CO_2 to hydrocarbons and alcohols and of N_2 to ammonia*, Department of Chemistry, Leiden University, The Netherlands, **March 2016**.
- *Electro-catalytic CO_2 and N_2 reduction*, Department of Physics, Technical University of Denmark (DTU), Lyngby, Denmark, **April 2015**.
- *Electrochemical reduction of N_2 and CO_2* , Department of Physics, Technical University of Denmark (DTU), Lyngby, Denmark, **June 2014**.
- *Predicting the mechanism and rate of electrochemical processes*, Department of Chemistry and Biochemistry, University of Iceland, Reykjavik, Iceland, **June 2013**.
- *Modeling electro-catalytic processes for energy conversion*, Department of Chemistry, Aalto University, Helsinki, Finland, **May 2013**.
- *Modeling active sites of nano-particles: H_2 formation and CO_2 reduction*, Department of Physics, Aalto University, Helsinki, Finland, **May 2013**.

- *Simulations of atomic scale transitions at charged interfaces*, Icelandic Center of Computational Science, **Oct 2009**.
- *Modeling Electro-catalytic Reactions using Density Functional Theory Calculations*, Department of Chemistry and Biochemistry, University of Iceland, Reykjavik, Iceland, **Aug 2009**.
- *Theoretical Calculations of Electrochemical Processes: Formation of Hydrogen Gas at Metal Electrodes*, Department of Chemistry and Biochemistry, University of Iceland, Reykjavik, Iceland, **Jan 2008**.

Oral Presentations for General Audience

- *Sustainable and green production of fuel and fertilizer for agriculture*, The Icelandic Physics Society, Reykjavík, Iceland, **April 2017**.
- *Sustainable production of fuel and fertilizer*, The Icelandic Chemical Society, Reykjavík, Iceland, **Oct 2015**.
- *Þróun rafefnahvata fyrir vistvæna og sjálfbæra eldsneytis- og áburðarframleiðslu (Development of electro-catalysts for green and sustainable fuel and fertilizer production)*, The Icelandic Research Fund's introduction meeting on "What are our scientists researching on?" Reykjavík, Iceland, **March 2015**.

Oral Presentations at Summer Schools or Ph.D. courses

- *Heterogeneous CO₂ reduction to fuel and N₂ reduction to ammonia*, NordCO₂ Autumn School: CO₂ conversion to fuel, Uppsala, Sweden, **Oct 2019**.
- *Heterogeneous CO₂ conversion*, NordCO₂ joint course: Mechanism for CO₂ activation, Tromso, Norway, **Sep 2018**.
- *DFT applications in electrochemistry*, Modeling methods in computational chemistry: theory and applications, Reykjavík, Iceland, **July 2016**.
- *Theoretical modeling*, Materials for the Hydrogen Society, Reykjavík, Iceland, **June 2013**.
- *Electrolysis*, Materials for the Hydrogen Society, Reykjavík, Iceland, **Aug 2010**.