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Hannes Jónsson

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ResearcherID: G-2267-2013

Education:

University of Iceland	B.S. in Chemistry	1980
University of California San Diego	Ph.D. Chemical Physics	1985
Dissertation: 'Quantum Mechanical Atom Scattering from Adsorbates at High and Low Coverage'		
Stanford University	Postdoctoral researcher	1986-1988
Research: Computer simulations of glass transition		

Employment:

University of Washington, Seattle	Assistant/Associate Professor	1988-1999
University of Washington, Seattle	Professor	1999-2005
University of Iceland, Reykjavík	Professor	2000-
Aalto University, Espoo	Finland Distinguished Prof.	2013-2016

Professional Affiliations:

Pacific NW Natl. Lab., Richland	Affiliate Staff Scientist	1994-2000
Physics Dpt., U. Washington, Seattle	Adjunct Associate Professor	1994-2005
Mat. Sci. & Eng. Dpt., UW Seattle	Adjunct Associate Professor	1994-2005
Tech. U. of Denmark, Physics Dpt.	Visiting Professor	1995-1996
Tech. U. of Denmark, Physics Dpt.	Visiting Professor	2004
Brown University, Providence	Adjunct Professor	2005-
SLAC, Stanford, California	Visiting Professor	2010
Aalto U., Dpt of Appl. Phys., Espoo	Visiting Professor	2011-2012
Ulam Scholar, CNLS, Los Alamos	Visiting Professor	2017-2018
DTU Dpt. of Energy Conv & Storage	Otto Mønsted Guest Professor	2018
Aalto U., Dpt of Appl. Phys., Espoo	Adjunct Professor	2018-

Publication Record:

Total number of citations is > 36000, thereof 4500 in year 2018,
according to Google Scholar, H-index = 55.
ISI WoS lists > 25000 citations and H-index of 48.
ResearcherID lists > 220 publications.

A complete list of articles and most manuscripts are available at *www.hi.is/∼hj*

Research supervision:

At the University of Washington (1988-2007):

Main supervisor of 12 Ph.D. students, co-advisor of 2 Ph.D. students.
Additional 4 students completed an M.S. degree.
7 postdoctoral associates worked in the research group.

At the University of Iceland (2000-):

Main supervisor of 10 Ph.D. students and 10 M.S. students that have graduated, and 11 post-docs that have moved on.
Currently supervising 4 and co-supervising 5 Ph.D. students, and 3 post-docs.

At Brown University (2005-):

Co-supervisor of one Ph.D. student that has graduated,
and one post-doc that has moved on,
currently co-supervising two Ph.D. students.

At Aalto University (2013-):

Co-supervisor of one Ph.D. student that has graduated and three post-docs who have moved on, currently co-supervising one Ph.D. student.

Teaching (at U. Washington, U. Iceland, Brown Univ. and Aalto Univ.):

First year chemistry (regular and honors) lectures and lab (U.W.)	1990-2005
Physical chemistry in B.S. chemistry program (U.W. and U.I.)	1992-2009
Quantum mechanics for graduate students in chemistry (U.W.)	1990-2000
Quantum mechanics for chemical engineering students (U.I.)	2015-2016
Thermodynamics and stat. mech. for phys. & chem. students (U.I.)	2007-2016
Computational chemistry for graduate students (U.I.)	2007-2013
Computational chemistry for graduate students (Brown U.)	2010-2011
Rate theory and long time scale simulations (Aalto Univ.)	2012

Organization of Symposia, Workshops and Summer Schools (past five years):

Summer school on 'New Materials for the Hydrogen Society'
Reykjavík, Iceland, June 2008
International Symposium on Metal Hydrogen Systems (MH2008)
Reykjavík, Iceland 2008
Summer school on 'New Materials for the Hydrogen Society'
Reykjavík, Iceland, August 2010
Symposium on 'Atomic-Scale Simulations' at the Para2010 conference
Reykjavík, Iceland, June 2010
Summer school on 'New Materials for the Hydrogen Society, Solar Fuel'
Reykjavík, Iceland, June 2013
Workshop on 'Magnetism in nanostructures'
Aalto Univ., Espoo, Finland, April 2014
Workshop on 'Nanomagnetism'
Reykjavík, Iceland, April 2015
Symposium on 'Advanced Atomistic Algorithms in Materials Science'

(co-organizer) MRS meeting, Boston, USA, November 2015
Symposium on 'Advanced Atomistic Algorithms in Materials Science'
(co-organizer) MRS meeting, Boston, USA, November 2017
Conference on 'Rate Theory and Long Time Scale Simulations'
(main organizer), Santa Fe, May 2018
International Workshop on Computational Electrochemistry
(co-organizer), Aalto University, July 2018
Symposium on 'Advances in Nanoparticles'
(co-organizer), E-MRS meeting in Warsaw, Sept. 2018

Honors and awards:

Otto Mønsted Guest Professor at Technical University of Denmark	2018
Stanislaw M. Ulam Scholar at CNLS, Los Alamos Nat. Lab.	2017-2018
Distinguished Guest Professor, Dpt. of Physics, USTC, Hefei, China	2016
Research excellence award, University of Iceland	2015
Computational Science Teaching Award of US Department of Energy	1995
ACCESS award for innovative development in undergraduate teaching, Univ. of Washington	1994
Fullbright Graduate Fellowship	1980

Editorial boards (current):

'Nanosystems: Physics, Chemistry, Mathematics'	2012-

Service (at Univ. of Iceland):

Science Institute of U. of Iceland	Director of Chemistry Division	2003-11
U. of Iceland, Financial committee	Representative of Sci. & Eng.	2007-09
Teaching Committee, Chairman	Physical and Natural Sci. Dpt.	2007-08
Science Institute, Univ. of Iceland	Chairman, Phys. Sciences Div.	2007-08

Other science related service (past 5 years):

Icelandic Research Fund, alternate on the five member board	2006-09
Icelandic Research Fund, on the five member board	2009-12
Danish Council for Independent Research / Natural Sciences (FNU) member of Chemistry panel	2011-13
Coordinator of 'Nordic-Russian Training Network on Nanomagnetism'	2013-15
German Research Fund (DFG), review panel for Solar Fuel SPP	2015
On advisory board of DOE funded 'Exascale Catalytic Chemistry'	2018-

Invited Research Presentations (past five years):

2014:

Workshop on 'Towards reality in Nano-scale Materials VII', Levi, Finland
'8th International Symposium on Hydrogen and Energy', Guangzhou, China
Technical University of Denmark, Physics Department, Lyngby, Denmark
Workshop on Aberration Corrected STEM, Borgarnes, Iceland

Dpt. of Chemistry, Jyvaskyla University, Finland
CECAM/COST workshop on Reducible Oxides, Zaragoza, Spain
'Workshop on reactivity and Catalysis of Metallic Nanoclusters', Espoo, Finland
'Electronic devices and materials at the nano-scale', Copenhagen, Denmark
'CAMD summer school on Electr. Structure Theory and Materials Design', Lyngby
'From chemical bond to chemical reactor: Comptnl. and Mtrls. challenges', India
'Atomic Scale Modelling of Materials', Lausanne, Switzerland
University of Helsinki, Dept. of Chemistry, Finland

2015:

Workshop on 'Towards reality in Nano-scale Materials VIII', Levi, Finland
Centre of Excellence in Computational Nanoscience, Aalto U., Finland
Sapienza University, Dept. of Physics, Rome, Italy
International Conference on Computational Science, Reykjavík, Iceland
2nd Int. Conf. on Nanotech., Nanomat. & Thin Films for Energy Applications, UK
Workshop on Nanocluster Structure and Catalysis, Birmingham, UK
Chalmers University, Physics Dpt., Gothenburg, Sweden
University College London, Chemical Engineering Dpt., London, UK
MRS Fall mtng, Symp. on 'Advanced Atomistic Algorithms in Matrls Sci', Boston, USA
Brown University, Chemistry Department, Providence, USA

2016:

American Chemical Society meeting, San Diego, USA
Physics Department, Temple University, USA
Workshop on Nanoclusters, Okinawa Instititute of Sci. and Tech., Japan
Department of Physics, University of Science and Technology, Hefei, China
Department of Chemistry, University of Science and Technology, Hefei, China
Fukui Institute of Theoretical Chemistry, Kyoto, Japan
Bridging Time Scale in Atomistic Computations, Dresden, Germany
Faraday Discussion on Rate Theory, Cambridge, UK
Molecules in Motion (MOLIM) 2016, Helsinki, Finland
Autumn School in Computational Physics, Helsinki, Finland

2017:

Center for Nonlinear studies (January), Los Alamos National Lab., NM, USA
Workshop on 'Towards reality in Nano-scale Materials VIII', Levi, Finland
Low Temperature Physics Lab., Aalto University, Espoo, Finland
High Performance Computing Workshop, Univ. of Iceland, Iceland
11th Congress of World Assoc. Theor. and Comp. Chemists, Munich, Germany
Center for Nonlinear studies (September), Los Alamos National Lab., NM, USA
University of New Mexico, ChemE and Chem. Dpt. colloq., NM, USA
Sandia National Laboratories (2 presentations), Albuquerque, NM, USA
MRS Fall mtng, Symp. on 'Advanced Atomistic Algor. in Matrls Sci', Boston, USA

2018:

ITMO University, Physics Dpt., St. Petersburg, Russia
12th Intl. Symposium Hydrogen & Energy, Lausanne, Switzerland
Copenhagen University, Dpt. of Chemistry, Copenhagen, Denmark

Aarhus University, Dpt. of Chemistry, Aarhus, Denmark
Shell Research Center, Amsterdam, The Netherlands
Conference on 'Rate Theory and Long Time Scale Simulations', Santa Fe, USA
CIMTEC Conference, Forum on New Materials, Perugia, Italy
Univ. of Bucharest, Dpt. of Organic Chemistry, Rumania
Interntl. Workshop on Computational Electrochemistry, Finland
American Chemical Society fall meeting, Boston, USA
'CAMD summer school on Electr. Structure Theory and Materials Design', Denmark
E-MRS meeting in Warsaw, Sept. (3 oral presentations)

2019 (so far):

Sanibel meeting St. Simon Island, Georgia, USA
Dpt. of Physics, Tulane Univ., New Orleans, USA
Institute for Computational Engineering and Sciences, UT Austin, USA
CECAM workshop on 'Carbon Materials', Helsinki, Finland
Dpt. of Chemistry, Univ. of Washington, Seattle, USA
Pacific Northwest National Lab, Richland, USA
Workshop on quantum materials, Reykjavík, Iceland

Publications (2017-):

Number of citations is > 36000 in Google Scholar, H-index = 55.
List of articles and links to most reprints/manuscripts is at http://www.hi.is/∼hj

Maxime Van den Bossche, Christoph Rose-Petruck, and Hannes Jónsson, 'Calculations of HCOOH formation in CO_2 electroreduction on Cu', (submitted).

M. J. Kolb, A. L. Garden, C. Badan, E. Skúlason, L. B.F. Juurlink, H Jónsson and M. T. M. Koper, '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', (submitted).

M. N. Potkina, I. S. Lobanov, O. A. Tretiakov, H. Jónsson and V. M. Uzdin, 'Antiskyrmions in Ferromagnets and Antiferromagnets: Stability and Dynamics', (submitted). Manuscript available on arXiv.

S. M. Vlasov, P.F. Bessarab, I. S. Lobanov, M. N. Potkina, V. M. Uzdin and H. Jónsson, 'Calculations of Magnetic Skyrmion Annihilation by Quantum Mechanical Tunneling', (submitted). Manuscript available on arXiv.

G.Levi, E. Biasin, A. Dohn, and H. Jónsson, 'On the Role of Solvent and Methyl Substituents in the Excited-State Dynamics of a Copper Phenanthroline Photosensitizer', (submitted).

A.V. Ivanov, V.M. Uzdin and H. Jónsson, 'Fast and Robust Algorithm for the Minimisation of the Energy of Spin Systems', (submitted). Manuscript available on arXiv.

G.P. Müller, M. Hoffmann, C. Disselkamp, D. Schürhoff, S. Mavros, M. Sallermann, N.S. Kiselev, H. Jónsson and S. Blügel, (submitted). 'Coupled quasimonopoles in chiral magnets', (submitted). Manuscript available on arXiv.

N.S. Kiselev, H. Jónsson and S. Blügel, 'Spirit: Multifunctional Framework for Atomistic Spin Simulations', G.P. Müller, M. Hoffmann, C. Disselkamp, D. Schrhoff, S. Mavros, M. Sallermann, *Phys. Rev. B* **99**, 224414 (2019).

Nicolai R. Mathiesen, Hannes Jónsson, Tejs Vegge and Juan Maria García Lastra, 'R-NEB: Accelerated nudged elastic band calculations by use of reflection symmetry', *J. Chem. Theo. Comput.* **15**, 3215 (2019).

Maxime Van den Bossche, Egill Skúlason, Christoph Rose-Petruck and Hannes Jónsson, 'Addition to "Assessment of Constant-Potential Implicit Solvation Calculations of Electrochemical Energy Barriers for H2 Evolution on Pt"', *J. Phys. Chem. C*, jpcc.9b05026

Maxime Van den Bossche, Egill Skúlason, Christoph Rose-Petruck and Hannes Jónsson, 'Assessment of constant-potential implicit solvation calculations of electrochemical energy barriers', *J. Phys. Chem C* **23**, 4116 (2019).

M. Geng and H. Jónsson, 'Density functional theory calculations and thermodynamic analysis of the forsterite Mg_2SiO_4(010) surface', *J. Phys. Chem C* **123**, 464 (2019).

E. Maras, M. Saito, K. Inoue, H. Jónsson, Y. Ikuhara and K. P. McKenna, 'Determination of the structure and properties of an edge dislocation in rutile TiO_2', *Acta Materialia* **163**, 199 (2019).

Ming Geng and Hannes Jónsson, 'Density functional theory calculation and thermodynamic analysis of the bridgmanite surface structure', *Phys. Chem. Chem. Phys.* **21**, 1009 (2019).

Unnar B. Arnalds, Sergi Y. Liashko, Pavel F. Bessarab, Valery M. Uzdin and Hannes Jónsson, 'Models of the energy landscape characterizing an element of a shakti spin lattice', *Nanosystems: Physics, Chemistry Mathematics* **9**, 711 (2018).

Xinxin Cheng, Elvar Jónsson, Hannes Jónsson and Peter M. Weber, 'Reply to "The Diamine Cation Is Not a Chemical Example Where Density Functional Theory Fails"', *Nature Communications* **9**, 5348 (2018).

G. P. Müller, P.F. Bessarab, S. M. Vlasov, F. Lux, N. S. Kiselev, V. M. Uzdin, S. Blügel and H. Jónsson, 'Duplication, collapse and escape of magnetic skyrmions revealed using a systematic saddle point search method', *Phys. Rev. Letters* **121**, 197202 (2018).

V. Ásgeirsson and H. Jónsson, 'Exploring potential energy surfaces with saddle point searches', chapter in the *Handbook of Materials Modeling.* Volume 1 "Methods: Theory and Modeling" (Springer, 2018).

G. Henkelman, H. Jónsson, T. Leliévre, N. Mousseau and A. Voter, 'Long-timescale simulations: challenges, pitfalls, best practices, for development and applications', chapter in the *Handbook of Materials Modeling.* Volume 1 "Methods: Theory and Modeling" (Springer, 2018).

A.L. Garden, A. Pedersen and H. Jónsson, 'Reassignment of "magic numbers" for Au clusters of decahedral and FCC structural motifs', *Nanoscale* **10**, 5124 (2018).

J. Hussain, H. Jónsson and E. Skúlason, 'Calculations of the rate of hydrocarbon and alcohol formation in CO_2 electroreduction', *ACS Catalysis* **8**, 5240 (2018).

P. F. Bessarab, G. P. Müller, I. S. Lobanov, F. N. Rybakov, N. S. Kiselev, H. Jónsson, V. M. Uzdin, S. Blügel, L. Bergqvist and A. Delin, 'Skyrmions in racetracks: Annihilation mechanisms and lifetime', *Scientific Reports* **8**, 3433 (2018).

V. M. Uzdin, M. N. Potkina, I. S. Lobanov, P. F. Bessarab, H. Jónsson, 'The effect of confinement and defects on the thermal stability of skyrmions', *Physica B* **549**, 6 (2018).

V.M. Uzdin, M.N. Potkina, I.S. Lobanov, P.F. Bessarab, H. Jónsson, 'Energy surface and lifetime of magnetic skyrmions', *Journal of Magnetism and Magnetic Materials* **459**, 236 (2018).

V. Ásgeirsson, A. Arnaldsson and H. Jónsson, 'Efficient evaluation of atom tunneling combined with electronic structure calculations', *J. Chem. Phys.* **148**, 102334 (2018).

S. Y. Liashko, H. Jónsson and V.M. Uzdin, 'Calculations of switching field and energy

barrier for magnetic islands with perpendicular anisotropy', *Nanosystems: Physics, Chemistry, Mathematics* **8**, 701 (2017).

S.M. Vlasov, P.F. Bessarab, V.M. Uzdin and H. Jónsson, 'Instantons describing tunneling between magnetic states at finite temperature', *Nanosystems: Physics, Chemistry, Mathematics* **8**, 746 (2017).

S.M. Vlasov, P.F. Bessarab, V.M. Uzdin and H. Jónsson, 'Nanocluster structure deduced from AC-STEM images coupled to theoretical modelling', K. Sukuta, M. V. d. Bossche, A. Pedersen and H. Jónsson, *Nanosystems: Physics, Chemistry, Mathematics* **8**, 723 (2017).

A. O. Dohn, E. Ö. Jónsson, G. Levi, J. J. Mortensen, O. Lopez, K. W. Jacobsen, K. B. Møller and H. Jónsson, 'A Real-Space Grid Implementation of QM/MM Electrostatic Embedding and Application to a Solvated Diplatinum Complex', *J. Chem. Theo. Comput.* 13, 6010 (2017).

S. Y. Liashko, I.S. Lobanov, V.M. Uzdin and H. Jónsson, 'Thermal stability of magnetic states in submicron magnetic islands', *Nanosystems: Physics, Chemistry, Mathematics* **8**, 572 (2017).

I.S. Lobanov, M.N. Potkina, H. Jónsson and V.M. Uzdin, 'Truncated minimum energy path method for finding first order saddle points', *Nanosystems: Physics, Chemistry, Mathematics* **8**, 586 (2017).

S. Smidstrup, D. Stradi, J. Wellendorff, P.A. Khomyakov, U.G. Vej-Hansen, M-E. Lee, T. Ghosh, E. Jónsson, H. Jónsson, K. Stokbro, 'First-principles Green's-function method for surface calculations: a pseudopotential localized basis set approach', Phys. Rev. B **96**, 195309 (2017).

S. Y. Liashko, H. Jónsson and V. M. Uzdin, 'The effect of temperature and external magnetic field on transitions in a kagome spin ice hexamer', *New Journal of Physics* **19**, 113008 (2017).

Y. Zhang, H. Jónsson and P. M. Weber, 'Coherence in Nonradiative Transitions: Internal Conversion in Rydberg-Excited N-Methyl and N-Ethyl Morpholine', *Physical Chemistry Chemical Physics* **19**, 26403 (2017).

Y. Jiao, B. W. Adams, A. O. Dohn, K. B. Møller, H. Jónsson, C. Rose-Petruck, 'Ultrafast X-ray Absorption Study of Longitudinal-Transverse Phonon Coupling in Electrolyte Aqueous Solution', *Phys. Chem. Chem. Phys.* **19**, 27266 (2017).

E. Maras, L. Pizzagalli, T. Ala-Nissila and H. Jónsson, 'Atomic Scale Formation Mechanism of Edge Dislocation Relieving Lattice Strain in a GeSi overlayer on Si(001)', *Scientific Reports* **7**, 11966 (2017).

S.M. Vlasov, P.F. Bessarab, V.M. Uzdin and H. Jónsson, 'Calculations of the onset temperature for tunneling in multispin systems', *Nanosystems: Physics, Chemistry, Mathematics* **8**, 454 (2017).

A. Ivanov, P. F. Bessarab, V. M. Uzdin and H. Jónsson, 'Magnetic exchange force microscopy: Theoretical analysis of induced magnetization reversals', *Nanoscale* **9**, 13320 (2017).

O-P. Koistinen, F. B. Dagbjartsdóttir, A. Vehtari and H. Jónsson. 'Nudged Elastic Band Calculations Accelerated with Gaussian Process Regression', *J. Chem. Phys.* **147**, 152720 (2017).

Y. Zhang, S. Deb, H. Jónsson and P. M. Weber, 'An Observation of Structural Wavepacket Motion: the Umbrella Mode in Rydberg-Excited N-Methyl Morpholine', *J. Phys. Chem. Letters* **8**, 3740 (2017).

S. Y. Liashko, V. M. Uzdin and H Jónsson, 'Energy surface and transition rates in a hexagonal element of spin ice', *Journal of Physics: Conf. Ser.* **903**, 012006 (2017).

A. Pedersen, L. Pizzagalli and H. Jónsson, 'Optimal atomic structure of amorphous silicon obtained from density functional theory calculations', *New Journal of Physics* **19**, 063018 (2017).

E. Skúlason and H. Jónsson, 'Atomic scale simulations of heterogeneous electrocatalysis: Recent advances', *Advances in Physics X* **2**, 481 (2017).

E. Ö. Jónsson, S. Lehtola, M. J. Puska and H. Jónsson, 'Theory and Applications of generalized Pipek–Mezey Wannier Functions', *J. Chem. Theo. Comput.* **13**, 460 (2017).

V. Ásgeirsson, H. Jónsson and K.Th. Wikfeldt, 'Long-timescale simulations of tunneling-assisted diffusion of hydrogen on ice surfaces at low temperature', *J. Phys. Chem. C.* **121**, 1648 (2017).

M.P. Gutiérrez, C. Argáez and H. Jónsson, 'Improved Minimum Mode Following Method for Finding First Order Saddle Points', *J. Chem. Theo. Comput.* **13**, 125 (2017).