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Hannes Jónsson

School of Engineering and Natural Sciences, Faculty of Physical Sciences
University of Iceland, VR-III, 107 Reykjavík, Iceland

E-mail: hj@hi.is *Web page: https://hj.hi.is*

ORCID: 0000-0001-8285-5421 *ResearcherID: G-2267-2013* *Scopus: ID:22971441100*

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	2005-2023
SLAC, Stanford, California	Visiting Professor	2010
Aalto U., Dpt of Appl. Phys., Espoo	Visiting Professor	2011-2012
Cntr. Non-linear Studies, Los Alamos	Ulam Scholar	2017-2018
DTU Dpt. of Energy Conv & Storage	Otto Mønsted Guest Professor	2018
Aalto U., Dpt of Appl. Phys., Espoo	Adjunct Professor	2018-2023

Publication Record:

Google Scholar lists $> 70\,000$ citations, thereof > 8000 in year 2023, h-index = 70, i10-index = 200.

Scopus lists $> 60\,000$ citations, h-index=61.

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 researchers worked in the research group.

At the University of Iceland (2000-):

Main supervisor of 16 and co-supervisor of 2 Ph.D., and 14 M.S. students that have graduated, as well as 13 postdoctoral researchers that have moved on. Currently supervising 6 and co-supervising 2 Ph.D. students, 1 M.S. student and 2 postdoctoral researchers.

At Brown University (2005-):

Co-supervisor of 3 Ph.D. students that have graduated, and one postdoctoral researcher that has moved on.

At Aalto University (2013-):

Co-supervisor of 2 Ph.D. students that have graduated and 3 postdoctoral researchers who have moved on.

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.)	2007-2022
Computational chemistry for graduate students (U.I.)	2007-2022
Computational chemistry for graduate students (Brown U.)	2010-2011
Rate theory and long time scale simulations (Aalto Univ.)	2012
Spectroscopy and reaction mechanism (U.I.)	2023

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

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
SciCADE International Conference on Scientific Computing (co-organizer), meeting in Reykjavík, July	2022
Lorentz Center / CECAM workshop on Electrochemistry (co-organizer), Leiden, The Netherlands, Jan.	2024

Honors and awards:

Van Arkel Honorary Professor of Chemistry, Leiden U., The Netherlands	2024
Stanislaw M. Ulam Scholar at CNLS, Los Alamos Nat. Lab., USA	2017-18
Otto Mønsted Guest Professor at Technical University of Denmark	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
Fulbright Graduate Fellowship	1980

Editorial boards:

'Langmuir' (an ACS journal on surface science)	1997-00
'Surface Science' (an Elsevier journal)	2004-09
'Nanosystems: Physics, Chemistry, Mathematics' (open source journal)	2012-
'Crystals' (open source journal)	2020-
'Magnetochemistry' (open source journal)	2020-

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-
Icelandic Infrastructure Fund, on the five member board	2019-22
Member of ERC stg. panel 'PE8: Product and Process Engineering'	2019-20
Member of ERC stg. panel 'PE4: Chemistry and Chemical Analysis'	2021-22

Research Presentations (past five years):

2019:

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

Summer School on Rare Events: Applications, Computation & Theory, Bangalore, Indi
Dpt. of Energy, Technical University of Milan, Italy
American Chemical Society conference, San Diego, USA (3 oral presentations)
CECAM50 conference, Lausanne, Switzerland
EPFL, Institute of Chemical Sciences and Engineering, Valais/Wallis, Switzerland
Quo Vadis Self-interaction Correction, Freiberg, Germany
American Vacuum Society conference, Columbus, USA
Materials Research Society fall meeting, Boston, USA

2020:

American Chemical Society fall meeting, (two on-line presentations)

2021:

Dpt. of Chemistry, Trinity College Dublin, Ireland (on-line presentations)
Materials Research Society spring meeting, Seattle , USA (two on-line presentations)
American Chemical Society fall meeting, Atlanta, USA (two presentations)
CNRS Inst. for Multiscale Modeling, Toulouse, France
Materials Research Society fall meeting, Boston , USA (two on-line presentation)

2022:

African School on Electronic Structure (on-line presentation)
American Physical Society March meeting, Chicago, USA
American Chemical Society spring meeting, San Diego, USA
Workshop titled 'Astrochemistry Meets Surface Science', Aarhus, Denmark
Dpt. of Chemistry, Lanchaster University, UK (on-line presentation)
'MagnetismMeet' conference on magnetism (on-line presentation), Japan
Materials Research Society spring meeting, Honolulu, USA (three presentations)
Electrochemical Society meeting, Vancouver, Canada
NanoInnovation Conference, Rome, Italy
van Marum Colloquium, Chemistry Dept., Leiden University, The Netherlands
Chemistry Dept., University of Jyväskylä, Finland

2023:

American Physical Society March meeting, Las Vegas, USA (on-line presentation)
Workshop on 'KMC as a Tool for Understanding Catalytic Functn.', Berlin, Germany
Physics Dept., Politecnico di Torino, Italy
Chemistry Dept., Technical Univ. of Denmark (DTU)
Workshop on 'Trends in topological nanomagnetism', Linnaeus U., Kalmar, Sweden
ECOSS36 'European conf. on Surf. Sci.', Lodz, Poland
ISACC 2023: 11th Internl. Symp. 'Atomic Cluster Collisions', Hveragerdi, Iceland
Physics Dept., Univ. of Central Florida, Orlando, USA
Sanibel Symposium, St. Augustine, Florida, USA
10th Interntl. Conf. on 'Excited States in Electr, & Bio Nanomat.', Santa Fe, USA
SSbench: CECAM workshop on Saddle point Search algorithms, Toulouse, France
American Chemical Society fall meeting, San Francisco, USA (four presentations)
Materials Research Society fall meeting, Boston, USA (two presentations)

Publications (2017-):

List of articles and links to most reprints/manuscripts at https://hj.hi.is

S. Hanslin, H. Jónsson and J. Akola, 'Doping-induced enhancement of hydrogen evolution at MoS_2 electrodes', ChemPhysChem. (Invited manuscript for an issue honouring Jens K. Nørskov, submitted).

M. Sallermann, H. Schrautzer, P. Bessarab and H. Jónsson, 'Identification of mechanisms of magnetic transitions using an efficient method for converging on first order saddle points', Manuscript available on arXiv.

Y. L. A. Schmerwitz, N. O. Ollé, G. Levi and H. Jónsson, 'Saddle Point Search Algorithms for Variational Density Functional Calculations of Excited Electronic States with Self-Interaction Correction', *Association for Computing Machinery's (ACM's) Digital Library* (2014). Manuscript available on arXiv.

A. Goswami, A. Pena-Torres, E. Ö. Jónsson, S. A. Egorov, and H. Jónsson, 'Evidence of sharp transitions between octahedral and capped trigonal prism states of the solvation shell of Fe^{3+}(aq)', *J. Chem. Phys. Letters* (2024). Manuscript available on arXiv.

N. E. Powers-Riggs, B. O. Birgisson, S. L. Raj, *et al.*, 'Characterization of deformational isomerization potential and interconversion dynamics with ultrafast X-ray solution scattering', *Journal of the American Chemical Society* (2024). Manuscript available on ChemRxiv.

M. A. H. Christiansen, A. Pena-Torres, E. Ö. Jónsson, and H. Jónsson, 'Single Atom Substituents in Copper Surfaces May Adsorb Multiple CO Molecules', *J. Chem. Phys. Letters* (2024).

Y. L. A. Schmerwitz, V. Ásgeirsson and H. Jónsson, 'Improved Initialisation of Optimal Path Calculations Using Sequential Traversal over the Image Dependent Pair Potential Surface', *J. Chem. Theory Comput.* **20**, 155 (2024). Manuscript available on arXiv.

J. J. Mortensen, A. H. Larsen, M. Kuisma, A. V. Ivanov, *et al.*, 'GPAW: Open Python Package for Electronic-structure Calculations', *J. Chem. Phys.* **160**, 092503 (2024).

S. Hanslin, H. Jónsson and J. Akola, 'Sulfur-deficient Edges as Active Sites for Hydrogen Evolution on MoS_2', *Phys. Chem. Chem. Phys.* **25**, 32541 (2023). Open access.

A. E. Sigurdarson, Y. L. A. Schmerwitz, Dagrún K. V. Tveiten, G. Levi and H. Jónsson, 'Orbital-optimized Density Functional Calculations of Molecular Rydberg Excited States with Real Space Grid Representation and Self-Interaction Correction', *J. Chem. Phys., John P. Perdew festschrift* **159**, 214109 (2023). Manuscript available on arXiv.

A. V. Ivanov, Y. L. A. Schmerwitz, G. Levi and H. Jónsson, 'Electronic Excitations of the Charged Nitrogen-Vacancy Center in Diamond Obtained Using Time-Independent Variational Density Functional Calculations', *SciPost Physics* **15**, 009 (2023). Open access.

Y. L. A. Schmerwitz, G. Levi and H. Jónsson, 'Calculations of Excited Electronic States by Converging on Saddle Points Using Generalized Mode Following', *J. Chem. Theory*

Comput. **19**, 3634 (2023). Manuscript available on arXiv.

S. Hanslin, H. Jónsson and J. Akola, 'Is Doped MoS_2 Basal Plane an Efficient Hydrogen Evolution Catalyst? Calculations of Voltage-Dependent Activation Energy', *Phys. Chem. Chem. Phys.* **25**, 15162 (2023). Manuscript available on arXiv.

B. Kirchhoff, E. Ö. Jónsson, T. Jacob and H. Jónsson, 'On the Challenge of Obtaining an Accurate Solvation Energy Estimate in Simulations of Electrocatalysis', *Top. Catal.* **66**, 1244 (2023). Manuscript available on arXiv.

J. Kloppenburg, L. B. Pártay, H. Jónsson and M. A. Caro, 'A General-purpose Machine Learning Pt Interatomic Potential for an Accurate Description of Bulk, Surfaces and Nanoparticles', *J. Chem. Phys.* **158**, 134704 (2023). Manuscript available on arXiv.

M. Lyu, Z. Li, M. Van den Bossche, H. Jónsson and C. Rose-Petruck, 'Electric Field Induced Release of Guest Molecules from Clathrate Hydrates and Its Consequences for Electrochemical CO_2 Conversion', *Chem. Phys.* **568**, 111839 (2023). Manuscript available on ChemRxiv.

M. N. Potkina, I.S. Lobanov, H. Jónsson and V.M. Uzdin, 'Stability of Magnetic Skyrmions: Systematic Calculations of the Effect of Size from Nanometer Scale to Microns', *Phys. Rev. B* **107**, 184414 (2023). Manuscript available on arXiv.

M. Sallermann, H. Jónsson and S. Blügel, 'Stability of Hopfions in Bulk Magnets with Competing Exchange Interactions', *Phys. Rev. B* **107**, 104404 (2023). Manuscript available on arXiv.

S. Rasti, E. Ö. Jónsson, H. Jónsson and J. Meyer, 'New Insights Into the Volume Isotope Effect of Ice Ih From Polarizable Many-Body Potentials', *J. Phys. Chem. Letters* **13**, 11831 (2022). Open source.

H. Myneni, E. Ö. Jónsson, H. Jónsson and A. O. Dohn, 'Development of a Polarizable Force Field for Acetonitrile Based on a Single-center Multipole Expansion', *J. Phys. Chem. B* **126**, 9339 (2022). Manuscript available on ChemRxiv.

E. Ö. Jónsson, S. Rasti, M. Galynska, J. Meyer and H. Jónsson, 'Transferable Potential Function for Flexible H_2O Molecules Based on the Single Center Multipole Expansion', *J. Chem. Theory Comput.* **18**, 7528 (2022). Manuscript available on arXiv.

G. S. Sun and H. Jónsson, 'Kinetic Monte Carlo Simulation Studies of the Shape of Islands on Close-packed Surfaces', *Journal of the Electrochemical Society* **169**, 102503 (2022).

J. Kloppenburg, A. Pedersen, K. Laasonen, M. Caro and H. Jónsson, 'Reassignment of Magic Numbers for Icosahedral Au Clusters: 310, 564, 928 and 1426', *Nanoscale* **14**, 9053 (2022). Manuscript available on arXiv.

B. Kirchhoff, C. Jung, H. Jónsson, D. Fantauzzi and T. Jacob, 'Simulations of the Electrochemical Oxidation of Pt Nanoparticles of Various Shapes', *J. Phys. Chem. C* **126**, 6773 (2022). Manuscript available on arXiv.

Y. L. A. Schmerwitz, A. V. Ivanov, E. Ö. Jónsson, H. Jónsson and Gianluca Levi, 'Variational Density Functional Calculations of Excited States: Conical Intersection and Avoided

Crossing in Ethylene Bond Twisting', *J. Phys. Chem. Letters* **13**, 3990 (2022). Manuscript available on arXiv.

A. Pena-Torres, A. Ali and H. Jónsson, 'Indirect Mechanism of Au Adatom Diffusion on the Si(100) Surface', *Phys. Rev. B* **105**, 205411 (2022). Manuscript available on arXiv.

A. Ali and H. Jónsson, 'Mechanism of Interlayer Transport on a Growing Au(111) Surface: 2D vs. 3D Growth', *Surfaces and Interfaces* **105**, 205411 (2022).

M. N. Potkina, I. S. Lobanov, H. Jónsson and V. M. Uzdin, 'Lifetime of Skyrmions in Discrete Systems with Infinitesimal Lattice Constant', *Journal of Magnetism and Magnetic Materials* **549**, 168974 (2022). Manuscript available on arXiv.

Z. Li, M. Lyu, H. Jónsson and C. Rose-Petruck, 'Observation of Electric-Field-Induced Liberation of Guest Molecules From Clathrate Hydrate', *J. Phys. Chem. Letters* **12**, 10410 (2021).

B. Kirchhoff, E. Ö. Jónsson, A. O. Dohn, T. Jacob and H. Jónsson, 'Elastic Collision Based Dynamic Partitioning Scheme for Hybrid Simulations', *J. Chem. Theory Comput.* **17**, 5863 (2021). Manuscript available on arXiv.

B. Kirchhoff, A. Ivanov, E. Sklason, D. Fantauzzi, T. Jacob and H. Jónsson, 'Assessment of the Accuracy of Density Functionals for Calculating Oxygen Reduction Reaction on Nitrogen Doped Graphene', *J. Chem. Theory Comput.* **17**, 6405 (2021). Manuscript available on arXiv.

V. Ásgeirsson, B. O. Birgisson, R. Bjornsson, U. Becker, F. Neese, C. Riplinger and H. Jónsson, 'Nudged elastic band method for molecular reactions using energy-weighted springs combined with eigenvector following', *J. Chem. Theory Comput.* **17**, 4929 (2021). Manuscript available on arXiv.

A. V. Ivanov, G. Levi, E. Ö. Jónsson and H. Jónsson, 'Method for Calculating Excited Electronic States Using Density Functionals and Direct Orbital Optimization with Real Space Grid or Plane-Wave Basis Set', *J. Chem. Theo. Comput.* **17**, 5034 (2021). Manuscript available on arXiv.

A. V. Ivanov, T. Ghosh, E. Ö. Jónsson and H. Jónsson, 'Mn Dimer can be Described Accurately with Density Functional Calculations when Self-interaction Correction is Applied' *J. Phys. Chem. Letters* **12**, 4240 (2021). Manuscript available on arXiv.

A. V. Ivanov, E. Ö. Jónsson, T. Vegge and H. Jónsson, 'Direct Energy Minimization Based on Exponential Transformation in Density Functional Calculations of Finite and Extended Systems', *Comp. Phys. Commun.* **267**, 108047 (2021). Manuscript available on arXiv.

M. Van den Bossche, C. Rose-Petruck and H. Jónsson, 'Competing HCOOH and CO Pathways in CO_2 Electroreduction at Copper Electrodes: Calculations of Voltage Dependent Activation Energy', *J. Phys. Chem. C* **125**, 13802 (2021).

M. Galynska, V. Ásgeirsson, H. Jónsson and R. Björnsson, 'Localized and Delocalized States of a Diamine Cation: Resolution of a Controversy', *J. Phys. Chem. Letters* **12**, 1250 (2021). Open access.

A. V. Ivanov, V. M. Uzdin and H. Jónsson, 'Fast and Robust Algorithm for the Energy Minimization of Spin Systems Applied in an Analysis of High Temperature Spin Configurations in Terms of Skyrmion Density', *Comp. Phys. Commun.* **260**, 107749 (2021). Manuscript available on arXiv.

G. Levi, A. V. Ivanov and H. Jónsson, 'Variational Density Functional Calculations of Excited States via Direct Optimization', *J. Chem. Theo. Comput.* **16**, 6968 (2020).

M. N. Potkina, I. S. Lobanov, O. A. Tretiakov, H. Jónsson and V. M. Uzdin, 'Stability of Long-lived Antiskyrmions in Mn-Pt-Sn Tetragonal Heusler Material', *Phys. Rev. B* **102**, 134430 (2020). 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', *New Journal of Physics* **22**, 083013 (2020). Open access.

E. Aprà, E. J. Bylaska, W. A. de Jong, *et al.* 'NWChem: Past, Present, and Future', *J. Chem. Phys.* **152**, 184102 (2020).

G. Levi, A. V. Ivanov and H. Jónsson, 'Variational Calculations of Excited States via Direct Optimization of the Orbitals in DFT', *Faraday Discussions* **224**, 448 (2020).

M. N. Potkina, I. S. Lobanov, H. Jónsson and V. M. Uzdin, 'Skyrmions in Antiferromagnets: Thermal Stability and the Effect of External Field and Impurities', *Journal of Applied Physics* **127**, 213906 (2020). 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, 'Coupled Quasimonopoles in Chiral Magnets', *Phys. Rev. B* **101**, 184405 (2020). Manuscript available on arXiv.

A. V. Ivanov, V. M. Uzdin and H. Jónsson, 'Efficient Optimization Method for Finding Minimum Energy Paths of Magnetic Transitions', *Journal of Physics: Condensed Matter* **32**, 345901 (2020). Manuscript available on arXiv.

A. V. Ivanov, P. F. Bessarab, V. M. Uzdin and H. Jónsson, 'Fully Self-consistent Calculations of Magnetic Structure Within Non-collinear Alexander-Anderson Model', *Nanosystems: Physics, Chemistry, Mathematics* **11**, 65 (2020). Open access.

A. Pedersen, L. Pizzagalli and H. Jónsson 'Atomic and Electronic Structure of a Vacancy in Amorphous Silicon', *Phys. Rev. B* **101**, 054204 (2020). 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', *Phys. Chem. Chem. Phys.* **22**, 748 (2020). Available at opinvisindi.is.

O-P. Koistinen, V. Ásgeirsson, A. Vehtari and H. Jónsson, 'Minimum Mode Saddle Point Searches Using Gaussian Process Regression with Inverse-distance Covariance Function', *J. Chem. Theo. Comput.* **16**, 499 (2020). Manuscript available on ChemRxiv.

B. Kirchhoff, L. Braunwarth, H. Jónsson, D. Fantauzzi and T. Jacob, 'Simulations of the Oxidation and Degradation of Platinum Electrocatalysts', *Small* **15**, 1905159 (2019).

M. Melander and H. Jónsson, 'Effect of H adsorption on the Magnetic Properties of an Fe

Island on a W(110) Surface', *Phys. Rev. B* **100**, 174431 (2019).

E. Ö. Jónsson, A. O. Dohn and H. Jónsson, 'Polarizable Embedding with a Transferable H_2O Potential Function I: Formulation and Tests on Dimer', *J. Chem. Theo. Comput.* **15**, 6562 (2019). Manuscript available on ChemRxiv.

A. O. Dohn, E. Ö. Jónsson and H. Jónsson, 'Polarizable Embedding with aTransferable H_2O Potential Function II: Application to (H_2O)n Clusters and Liquid Water', *J. Chem. Theo. Comput.* **15**, 6578 (2019). Manuscript available on ChemRxiv.

O-P. Koistinen, V. Ásgeirsson, A. Vehtari and H. Jónsson, 'Nudged elastic band calculations accelerated with Gaussian process regression based on inverse inter-atomic distances', *J. Chem. Theo. Comput.* **15**, 6738 (2019). Manuscript available on ChemRxiv.

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', *Phys. Chem. Chem. Phys.* **21**, 17142 (2019).

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

N. R. Mathiesen, H. Jónsson, T. Vegge and J. M. García Lastra, 'R-NEB: Accelerated nudged elastic band calculations by use of reflection symmetry', *J. Chem. Theo. Comput.* **15**, 3215 (2019).

M. Van den Bossche, E. Skúlason, C. 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* **123**, 15875 (2019).

M. Van den Bossche, E. Skúlason, C. Rose-Petruck and H. 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).

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

U. B. Arnalds, S. Y. Liashko, P. F. Bessarab, V. M. Uzdin and H. Jónsson, 'Models of the energy landscape characterizing an element of a shakti spin lattice', *Nanosystems: Physics, Chemistry Mathematics* **9**, 711 (2018).

X. Cheng, E. Ö. Jónsson, H. Jónsson and P. 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).

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