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Professional experience

ETH Zurich — Zurich, Switzerland
Assistant Professor of Digital Chemistry — 2023–

University of Toronto/Chalmers University of Technology — Toronto, Canada
Postdoctoral researcher — 2021–2022
Project: “Inverse design of molecules and reactions”

AstraZeneca UK — Macclesfield, United Kingdom
Postdoctoral researcher — 2018–2020
Project: “Uniform quantitative predictive modelling for route design”

Education

Uppsala University — Uppsala, Sweden
Ph.D. Chemistry — 2013–2018
Thesis: “Influence of Aromaticity on Excited State Structure, Reactivity and Properties”

Uppsala University — Uppsala, Sweden
M.Sc. Chemistry — 2011–2013
Thesis: “Improving the norbornadiene/quadricyclane solar fuel system exploiting excited state aromaticity”

Uppsala University — Uppsala, Sweden
B.Sc. Chemistry — 2008–2011
Thesis: “Synthesis of donor-bridge-donor compounds for electron transfer studies”

Conferences and talks

Invited talks

Advances in N-body Computations — 2022
Oxford, United Kingdom. April 11-13

VISTA Symposium on Artificial-Intelligence and Data-Science Assisted Synthesis — 2021
Online. July 13-20

Oral presentations

Pacifichem. Computational Chemistry for Pharmaceutical Route Development — 2021
Online. December 16–21

AI for Reaction Outcome and Synthetic Route Prediction — 2020
Tortworth, United Kingdom. March 9–11

47th Physical Organic Minisymposium — 2019
York, Canada. November 1–3

1st National Meeting of the Swedish Chemical Society — 2018
Lund, Sweden. June 17–20

23rd IUPAC Conference on Physical Organic Chemistry — 2016
Sydney, Australia. July 3–6

Meeting on Molecular Solar Thermal Energy Storage Systems — 2016
Gothenburg, Sweden. April 21–22

Talks to organizations

EPFL — 2023–05–09
AI in Chemistry and beyond. Lausanne, Switzerland

ICIQ 2022–01–10
Tarragona, Spain

AstraZeneca 2021–11–24
Predictive Science Network. Online

ETH Zürich 2021-11-04
Mini-Symposium on Digital Chemistry. Online

IQ Consortium 2021–02–17
Computational Chemistry Work Group. Online

IBM Research 2020–10–20
Synthesis prediction group. Online

University of Warwick 2019–07–04
Warwick, United Kingdom. Department of Chemistry

Poster presentations

21st Tetrahedron Symposium 2021
Online. June 21–24

Chemical Science Symposium 2020 2020
Online. September 29–30

3rd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry 2020
Online. September 28–29

Computational Molecular Science 2019
Coventry, United Kingdom. March 27–29

Girona Seminar – Predictive Catalysis 2018
Girona, Spain. April 3–6

11th Triennial Congress of the World Association of Theoretical and Computational Chemistry 2017
Munich, Germany. August 27–September 1

Gordon Research Conference on Physical Organic Chemistry 2017
Holderness, NH, USA. June 25–30

8th Molecular Quantum Mechanics 2016
Uppsala, Sweden. June 26 – July 1

Gordon Research Conference on Physical Organic Chemistry 2015
Holderness, NH, USA. June 21–26

The Chemical Bonds at the 21st Century 2015
Xiamen, China. June 14–18

Swedish Theoretical Chemistry Meeting 2014 – New Horizons 2014
Uppsala, Sweden. October 27–29

XXVth IUPAC Symposium on Photochemistry 2014
Bordeaux, France. July 13–18

Workshops

Machine Learning for Molecules Workshop @ NeurIPS 2020
Online. December 12

9th RDKit User Group Meeting 2020
Online. October 6–8

The 8th MOLCAS users' Workshop 2017
Uppsala, Sweden. November 20–24

Workshop on Ab Initio Valence Bond theory 2015
Xiamen, China. June 16–18

Unconventional Solar Energy Technologies 2013
Gothenburg, Sweden. June 24–29

Exchanges

Xiamen University, China 2016
Group of Wei Wu. Ab initio valence bond calculations of excited states. September–October

Publications & software

Under review & pre-prints

(1) Nigam, A.; Pollice, R.; Tom, G.; Jorner, K.; Thiede, L. A.; Kundaje, A.; Aspuru-Guzik, A. Tartarus: A Benchmarking Platform for Realistic and Practical Inverse Molecular Design `http://arxiv.org/abs/2209.12487`, preprint.

(2) Yudin, A.; Apte, C.; Heller, N.; Marr, A.; Jorner, K.; Aspuru-Guzik, A. A Borindolizine Platform for the Design of Fluorophores with Tunable Emissions `https://chemrxiv.org/engage/chemrxiv/article-details/62e443d9cf6612a8c2badbdd`, preprint.

Articles

(1) Jorner, K. Putting Chemical Knowledge to Work in Machine Learning for Reactivity. *Chimia* **2023**, *77*, 22, DOI: 10.2533/chimia.2023.22.

(2) Jorner, K. Revisiting the Superaromatic Stabilization Energy as a Local Aromaticity Index for Excited States. *J. Phys. Org. Chem.* **2023**, *36*, e4460, DOI: 10.1002/poc.4460.

(3) Pablo-García, S.; Morandi, S.; Vargas-Hernández, R. A.; Jorner, K.; Ivković, Ž.; López, N.; Aspuru-Guzik, A. Fast Evaluation of the Adsorption Energy of Organic Molecules on Metals via Graph Neural Networks. *Nature Computational Science* **2023**, *3*, 433–442, DOI: 10.1038/s43588-023-00437-y.

(4) Stuyver, T.; Jorner, K.; Coley, C. W. Reaction Profiles for Quantum Chemistry-Computed [3 + 2] Cycloaddition Reactions. *Sci. Data* **2023**, *10*, 66, DOI: 10.1038/s41597-023-01977-8.

(5) Vargas–Hernández, R. A.; Jorner, K.; Pollice, R.; Aspuru–Guzik, A. Inverse Molecular Design and Parameter Optimization with Hückel Theory Using Automatic Differentiation. *J. Chem. Phys.* **2023**, *158*, 104801, DOI: 10.1063/5.0137103.

(6) Cao, Y.; Ser, C. T.; Skreta, M.; Jorner, K.; Kusanda, N.; Aspuru-Guzik, A. Reinforcement Learning Supercharges Redox Flow Batteries. *Nat. Mach. Intell.* **2022**, *4*, 667–668, DOI: 10.1038/s42256-022-00523-2.

(7) El Bakouri, O.; Szczepanik, D. W.; Jorner, K.; Ayub, R.; Bultinck, P.; Solà, M.; Ottosson, H. Three-Dimensional Fully π-Conjugated Macrocycles: When 3D-aromatic and When 2D-aromatic-in-3D? *J. Am. Chem. Soc.* **2022**, *144*, 8560–8575, DOI: 10.1021/jacs.1c13478.

(8) Gensch, T.; dos Passos Gomes, G.; Friederich, P.; Peters, E.; Gaudin, T.; Pollice, R.; Jorner, K.; Nigam, A.; Lindner-D'Addario, M.; Sigman, M. S.; Aspuru-Guzik, A. A Comprehensive Discovery Platform for Organophosphorus Ligands for Catalysis. *J. Am. Chem. Soc.* **2022**, *144*, 1205–1217, DOI: 10.1021/jacs.1c09718.

(9) Ayub, R.; El Bakouri, O.; Smith, J. R.; Jorner, K.; Ottosson, H. Triplet State Baird Aromaticity in Macrocycles: Scope, Limitations, and Complications. *J. Phys. Chem. A* **2021**, *125*, 570–584, DOI: 10.1021/acs.jpca.0c08926.

(10) Jorner, K.; Brinck, T.; Norrby, P.-O.; Buttar, D. Machine Learning Meets Mechanistic Modelling for Accurate Prediction of Experimental Activation Energies. *Chem. Sci.* **2021**, *12*, 1163–1175, DOI: 10.1039/D0SC04896H.

(11) Jorner, K.; Tomberg, A.; Bauer, C.; Sköld, C.; Norrby, P.-O. Organic Reactivity from Mechanism to Machine Learning. *Nat. Rev. Chem.* **2021**, *5*, 240–255, DOI: 10.1038/s41570-021-00260-x.

(12) Thakkar, A.; Johansson, S.; Jorner, K.; Buttar, D.; Reymond, J.-L.; Engkvist, O. Artificial Intelligence and Automation in Computer Aided Synthesis Planning. *React. Chem. Eng.* **2021**, *6*, 27–51, DOI: 10.1039/D0RE00340A.

(13) Jorner, K.; Rabten, W.; Slanina, T.; Proos Vedin, N.; Sillén, S.; Wu Ludvigsson, J.; Ottosson, H.; Norrby, P.-O. Degradation of Pharmaceuticals through Sequential Photon Absorption and Photoionization in Amiloride Derivatives. *Cell Rep. Phys. Sci.* **2020**, *1*, 100274, DOI: 10.1016/j.xcrp.2020.100274.

(14) Yadav, S.; El Bakouri, O.; Jorner, K.; Tong, H.; Dahlstrand, C.; Solà, M.; Ottosson, H. Exploiting the Aromatic Chameleon Character of Fulvenes for Computational Design of Baird-aromatic Triplet Ground State Compounds. *Chem. – Asian J.* **2019**, *14*, 1870–1878, DOI: 10.1002/asia.201801821.

(15) Jorner, K.; Jahn, B. O.; Bultinck, P.; Ottosson, H. Triplet State Homoaromaticity: Concept, Computational Validation and Experimental Relevance. *Chem. Sci.* **2018**, *9*, 3165–3176, DOI: 10.1039/C7SC05009G.

(16) Poon, J.-f.; Yan, J.; Jorner, K.; Ottosson, H.; Donau, C.; Singh, V. P.; Gates, P. J.; Engman, L. Substituent Effects in Chain-Breaking Aryltellurophenol Antioxidants. *Chem. - Eur. J.* **2018**, *24*, 3520–3527, DOI: 10.1002/chem.201704811.

(17) Ayub, R.; Bakouri, O. E.; Jorner, K.; Solà, M.; Ottosson, H. Can Baird's and Clar's Rules Combined Explain Triplet State Energies of Polycyclic Conjugated Hydrocarbons with Fused 4nπ- and (4n + 2)π-Rings? *J. Org. Chem.* **2017**, *82*, 6327–6340, DOI: 10.1021/acs.joc.7b00906.

(18) Ayub, R.; Jorner, K.; Ottosson, H. The Silacyclobutene Ring: An Indicator of Triplet State Baird-aromaticity. *Inorganics* **2017**, *5*, 91, DOI: 10.3390/inorganics5040091.

(19) Ayub, R.; Papadakis, R.; Jorner, K.; Zietz, B.; Ottosson, H. Cyclopropyl Group: An Excited-State Aromaticity Indicator? *Chem. - Eur. J.* **2017**, *23*, 13684–13695, DOI: 10.1002/chem.201701404.

(20) Jorner, K.; Dreos, A.; Emanuelsson, R.; El Bakouri, O.; Fdez. Galván, I.; Börjesson, K.; Feixas, F.; Lindh, R.; Zietz, B.; Moth-Poulsen, K.; Ottosson, H. Unraveling Factors Leading to Efficient Norbornadiene-Quadricyclane Molecular Solar-Thermal Energy Storage Systems. *J. Mater. Chem. A* **2017**, *5*, 12369–12378, DOI: 10.1039/C7TA04259K.

(21) Lundstedt, A.; Papadakis, R.; Li, H.; Han, Y.; Jorner, K.; Bergman, J.; Leifer, K.; Grennberg, H.; Ottosson, H. White-Light Photoassisted Covalent Functionalization of Graphene Using 2-Propanol. *Small Methods* **2017**, *1*, 1700214, DOI: 10.1002/smtd.201700214.

(22) Oh, J.; Sung, Y. M.; Mori, H.; Park, S.; Jorner, K.; Ottosson, H.; Lim, M.; Osuka, A.; Kim, D. Unraveling Excited-Singlet-State Aromaticity via Vibrational Analysis. *Chem* **2017**, *3*, 870–880, DOI: 10.1016/j.chempr.2017.09.005.

(23) Ueda, M.; Jorner, K.; Sung, Y. M.; Mori, T.; Xiao, Q.; Kim, D.; Ottosson, H.; Aida, T.; Itoh, Y. Energetics of Baird Aromaticity Supported by Inversion of Photoexcited Chiral [4n]Annulene Derivatives. *Nat. Commun.* **2017**, *8*, 346, DOI: 10.1038/s41467-017-00382-1.

(24) Jorner, K.; Feixas, F.; Ayub, R.; Lindh, R.; Solà, M.; Ottosson, H. Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. *Chem. - Eur. J.* **2016**, *22*, 2793–2800, DOI: 10.1002/chem.201504924.

(25) Papadakis, R.; Li, H.; Bergman, J.; Lundstedt, A.; Jorner, K.; Ayub, R.; Haldar, S.; Jahn, B. O.; Denisova, A.; Zietz, B.; Lindh, R.; Sanyal, B.; Grennberg, H.; Leifer, K.; Ottosson, H. Metal-Free Photochemical Silylations and Transfer Hydrogenations of Benzenoid Hydrocarbons and Graphene. *Nat. Commun.* **2016**, *7*, 12962, DOI: 10.1038/ncomms12962.

(26) Rudebusch, G. E.; Zafra, J. L.; Jorner, K.; Fukuda, K.; Marshall, J. L.; Arrechea-Marcos, I.; Espejo, G. L.; Ponce Ortiz, R.; Gómez-García, C. J.; Zakharov, L. N.; Nakano, M.; Ottosson, H.; Casado, J.; Haley, M. M. Diindeno-Fusion of an Anthracene as a Design Strategy for Stable Organic Biradicals. *Nat. Chem.* **2016**, *8*, 753–759, DOI: 10.1038/nchem.2518.

(27) Mohamed, R. K.; Mondal, S.; Jorner, K.; Faria Delgado, T.; Lobodin, V. V.; Ottosson, H.; Alabugin, I. V. The Missing C1-C5 Cycloaromatization Reaction: Triplet State Antiaromaticity Relief and Self-Terminating Photorelease of Formaldehyde for Synthesis of Fulvenes from Enynes. *J. Am. Chem. Soc.* **2015**, *137*, 15441–15450, DOI: 10.1021/jacs.5b07448.

(28) Jorner, K.; Emanuelsson, R.; Dahlstrand, C.; Tong, H.; Denisova, A. V.; Ottosson, H. Impact of Ground- and Excited-State Aromaticity on Cyclopentadiene and Silole Excitation Energies and Excited-State Polarities. *Chem. - Eur. J.* **2014**, *20*, 9295–9303, DOI: 10.1002/chem.201402577.

(29) Göransson, E.; Emanuelsson, R.; Jorner, K.; Markle, T. F.; Hammarström, L.; Ottosson, H. Charge Transfer through Cross-Hyperconjugated versus Cross-π-Conjugated Bridges: An Intervalence Charge Transfer Study. *Chem. Sci.* **2013**, *4*, 3522–3532, DOI: 10.1039/C3SC50844G.

(30) Hellström, M.; Jorner, K.; Bryngelsson, M.; Huber, S. E.; Kullgren, J.; Frauenheim, T.; Broqvist, P. An SCC-DFTB Repulsive Potential for Various ZnO Polymorphs and the ZnO–Water System. *J. Phys. Chem. C* **2013**, *117*, 17004–17015, DOI: 10.1021/jp404095x.

Books & chapters

(1) Jorner, K., Baird aromaticity in excited states and open-shell ground states In *Aromaticity: Modern Computational Methods and Applications*, Fernández, I., Ed.; Elsevier: Amsterdam, 2021; Chapter 12.