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RESEARCH PROFILE

Background

Chemistry — supramolecular, synthetic/physical organic (PhD, industry, post-doc)

Engineering — electrical/software (BSc, industry, post-doc)

Interests

Automated chemical discovery

Probabilistic/logic techniques in chemical/biomolecular space

Language, compilation, and inference applied to physical processes

EMPLOYMENT

Post-doctoral Research Assistant Cronin group, *University of Glasgow*, Glasgow, UK 2018–(2020)
Helped develop abstractions and software for universal digitization and robotic automation of chemical synthesis.

Specialist Drug Analysis Service, *Health Canada*, Burnaby, Canada 2017–2018
Designed and implemented a high-performance algorithm in *Julia* to automatically identify and measure drug molecules in mixtures using NMR spectroscopy.

EDUCATION

Doctor of Philosophy Chemistry, *University of British Columbia (UBC)*, Vancouver, Canada 2011–2017
Created materials with new and unusual properties by harnessing tautomerism and electron delocalization.
Supervisor: Prof. Mark MacLachlan

Bachelor of Science Electrical Engineering, *Sharif University of Technology*, Tehran, Iran 2005–2009
Used *finite-difference time-domain* methods to study light propagation in photonic crystals.
Supervisor: Prof. Khashayar Mehrany

PUBLICATIONS

A universal approach to the digitization and automatic execution of the chemical synthesis literature
Mehr, S. H. M.; Craven, M.; Leonov, A. I.; Keenan, G.; Cronin, L.
Nature, 2020 *(under review)*

Intuition-Enabled Machine Learning Beats the Competition When Joint Human-Robot Teams Perform Inorganic Chemical Experiments
Duros, V.; Grizou, J.; Sharma, A.; Mehr, S. H. M.; Bubliauskas, A.; Frei, P.; Miras, H. N.; Cronin, L.
J. Chem. Inf. Model., 2019 (DOI: 10.1021/acs.jcim.9b00304)

Catalyst: The Metaphysics of Chemical Reactivity
Cronin, L.; Mehr, S. H. M.; Granda, J. M.
Chem, **2018**, 4 (8), 1759–1761 (DOI: 10.1016/j.chempr.2018.07.008)

Controlling Ligand Exchange through Macrocyclization
Carta, V.; Mehr, S. H. M.; MacLachlan, M. J.
Inorganic chemistry, **2018**, 57 (6) 3243–3253 (DOI: 10.1021/acs.inorgchem.8b00031)

Turing the tautomeric behaviour of tris(salicylaldimines)
Mehr, S. H. M.; Oshima, H.; Carta, V.; Patrick, B. O.; White, N. G.; MacLachlan, M. J.
Org. Biomol. Chem, **2018**, 15 (39), 3243–3253 (DOI: 10.1039/C7OB02058A)

Formylation of phenols using formamidine acetate
Mehr, S. H. M.; Depmeier, H.; Fukuyama, K.; Maghami, M.; MacLachlan, M. J.
Org. Biomol. Chem., **2017**, 15 (3), 581–583 (DOI: 10.1039/C6OB02727J)

Stabilization of a Strained Heteroradialene by Peripheral Electron Delocalization
Mehr, S. H. M.; Patrick, B. O.; MacLachlan, M. J.
Org. Lett., **2016**, 18 (8), 1840–1843 (DOI: 10.1021/acs.orglett.6b00577)

Deuteration of Aromatic Rings Under Very Mild Conditions Through Keto-Enamine Tautomeric Amplification
Mehr, S. H. M.; Fukuyama, K.; Bishop, S.; Lelj, F.; MacLachlan, M. J.
J. Org. Chem, **2015**, 80 (10), 5144–5150 (DOI: 10.1021/acs.joc.5b00539)

Novel PPV/Mesoporous Organosilica Composites: Influence of the Host Chirality on a Conjugated Polymer Guest
Mehr, S. H. M.; Giese, M.; Qi, H.; Shopsowitz, K.; Hamad, W. Y.; MacLachlan, M. J.
Langmuir, **2013**, 29 (40), 12579–12584 (DOI: 10.1021/la4024597)

Role of Entropy and Autosolvation in Dimerization and Complexation of C_{60} by Zn_7 Metallocavitands
Frischmann, P.D.; Mehr, S. H. M.; Patrick, B. O.; Lelj, F.; MacLachlan, M. J.
Inorg. Chem., **2012**, 51 (6), 3443–3453 (DOI: 10.1021/ic202049t)

Influence of asymmetry on the band structure of photonic crystals
Mehr, S. H. M.; Khorasani, S.
in *OPTO*, International Society For Optics And Photonics, **2010**, 76091–76091 (DOI: 10.1117/12.839839)

PROPOSAL CONTRIBUTIONS

Exploration of Chemical Space with Autonomous Robots for Generating Knowledge CHEMTREK
ERC Advanced Grant, 2020–2025, **€ 2.5 M**

Molecular Automated Discovery of Novelty Enabled by Synthetic Systems (MADNESS)
DARPA Accelerated Molecular Discovery (AMD), 2019–2023, **$ 4 M**

TALKS AND POSTER PRESENTATIONS

Saving Lives with Julia
JuliaCon 2018, London, UK

Badass Bonding — Unsettled Electrons in Shape-Shifting Molecules
Inorganic Discussion Group, Department of Chemistry, 2016, UBC, Vancouver

A Switch in Character: Deriving Novel Reactivity from Tautomerism
ISMSC 2015: 10th International Symposium on Macrocyclic and Supramolecular Chemistry, 2015, Strasbourg

Kinetics by NMR: A Live Demonstration
8th Annual VIVA NMR Symposium, August, 2014, Vancouver

Using Tautomers for Gentle Deuteration of Benzene Rings
97th Canadian Chemistry Conference and Exhibition, June, 2014, Vancouver

Macrocycles as Functional Materials
Canada-Japan Joint Symposium on Supramolecular Nanomaterials Science, May, 2012, Whistler

AWARDS & HONOURS

ASPIRE Challenge NIH National Center for Advancing Translational Science, 2019

International Tuition Award UBC, 2011–2017

ISMSC Scholarship Competitive award for abstracts at the 10th International Symposium on Macrocyclic and Supramolecular Chemistry, Strasbourg, 2015

Arnold By Travel Award UBC, 2015

Graduate Student Travel Award UBC, 2015

Faculty of Science Graduate Award UBC, 2016–2017

Faculty of Science PhD Tuition Award UBC, 2016–2017

LEADERSHIP & PUBLIC ENGAGEMENT

Vice president Chemistry Graduate Student Society (CGSS), UBC, 2013–2014

Presenter/facilitator *Chemistry Field Trips* for high school students, UBC, 2012–2016

Presenter/facilitator *Chemistry Beyond the Magic* open house, UBC, 2011–2015

TEACHING EXPERIENCE

Shared Instrument Facility (TA) University of British Columbia (UBC), 2012–2016

Organic Chemistry Farzanegan High School, 2005–2010

Digital Signal Processing Lab (TA) Sharif University of Technology, 2009–2010

Chemistry for the International Chemistry Olympiad Allameh Helli High School, Tehran, Iran, 2004–2010

STUDENTS SUPERVISED

Hannah Depmeier Novel methods towards multiple-formylation of phenols 2016 (BSc)

Mahboobeh Maghami Tautomerism in Schiff base macrocycles 2014–2015 (PhD)

Stephanie Bishop Facile H/D exchange in salicylideneamine derivatives 2013–2014 (BSc)

Marcus Farnfield Salicylaldimines as photodegradable crosslinkers 2013–2014 (BSc)

Jason Yang Molecular capsules based on salicylaldimines 2013–2014 (BSc)

SKILLS

Programming Julia, Python, Prolog, Clojure, OCaml, C, Rust, JavaScript, LaTeX (`github.com/hessammehr`)

Analytical techniques NMR spectroscopy, MALDI-TOF mass spectrometry

Chemistry Organic synthesis, macrocycle and supramolecule design, *ab initio* computational chemistry