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Google Scholar: <https://scholar.google.com/citations?user=mOj8bIcAAAAJ&hl=en>

EDUCATION

Ph.D., 09/2005, **Princeton University**, Princeton, USA
Department of Mechanical and Aerospace Engineering
Dissertation: *Grain Boundary Migration in Metals: Molecular Dynamics Simulations*
Advisor: Professor David J. Srolovitz

M.Sc., 07/1999, **Tsinghua University**, Beijing, China
Department of Materials Science and Engineering
Thesis: *A Molecular Dynamics Simulation of Cluster Al Depositing on Si Substrate by Ionized Cluster Beam Method*
Advisor: Professor Zongning Xia

B.E., 07/1996, **Tsinghua University**, Beijing, China
Department of Materials Science and Engineering

PROFESSIONAL EXPERIENCE

Associate Dean Graduate Students (CME), University of Alberta, Canada,
07/01/2022 - present

Associate Chair Graduate Studies, Chemical and Materials Engineering,
University of Alberta, Canada, 07/01/2021 – 06/30/2022

Professor, University of Alberta, Canada, 07/01/2017 – present

Associate Professor, University of Alberta, Canada, 07/01/2013 – 06/30/2017

Assistant Professor, University of Alberta, Canada, 09/01/2007 – 06/30/2013

Research Associate, Princeton University, USA, 10/01/2005 – 08/15/2007

SABBATICAL

Visiting Professor, University of Science & Technology Beijing, China, 09/01/2013 – 06/30/2014

Visiting Professor, Zhejiang University, China, 02/25/2014 – 03/24/2014

RESEARCH INTERESTS

- Interfacial dynamics of nanoparticles
- Mechanical response in nanostructured materials
- Atomistic deformation mechanisms for metallic glasses
- Multiscale simulation of crack initiation and propagation in near neutral pH stress corrosion cracking
- Hydrogen embrittlement in iron
- ZnS nanoparticles phase transition
- High capacity of hydrotalcite for CO₂ capture
- Battery and energy storage materials
- High Entropy Alloys
- Nucleation and growth of calcite

SCHOLARSHIPS AND HONORS

- *Grain Boundaries Exhibit the Dynamics of Glass-Forming Liquids*, published in PNAS, was featured in Editor's Choice, Science, 324; 858, 2009
- Best Poster Award, Gordon Research Conference on Physical Metallurgy, 2006
- Guggenheim Fellowship, Princeton University, 2000
- Guanghua Fellowship, Tsinghua University, China, 1998

GRANTS AND AWARDS

- 07/10/2022 – 07/09/2026 NSERC Alliance Grants (w/Dr. Jing Liu, \$280,000, PI) Title: *Identifying the influence of environmental factors and steel surface conditions on hydrogen uptake under high-pressure hydrogen transportation*

and storage conditions

- 09/01/2022 – 03/31/2024 CME Research Seed Funding (w/Dr. Jing Liu, \$50,000, Co-PI)
Title: *Fabrication and Interpretation of High Entropy Alloy Nanoparticles as Electrocatalysts for Hydrogen Production*
- 04/01/2022 – 03/31/2027 NSERC Discovery Grant (\$165,000, PI)
Title: *Understanding of Hydrogen Embrittlement in Steels from Atomistic Perspective*
- 03/01/2022 – 02/29/2024 NSERC Alliance Grants (w/Dr. Zhi Li, \$200,000, Co-PI)
Title: *Scalable preparation of g-C₃N₄ nanosheets and quantum dots for metal anode protection and nitrogen reduction*
- 02/01/2022 – 06/30/2022 Faculty of Engineering Seed Funding (w/Dr. Jing Liu, \$50,000, Co-PI)
Title: *Comprehensive Investigation of Hydrogen Uptake in Pipeline Steels*
- 10/01/2021 – 03/31/2022 CanmetMATERIALS (CMAT) (\$ 23,000, PI)
Title: *Fundamental understanding of hydrogen uptake and its influence on pipeline structural integrity*
- 03/15/2021 – 03/14/2024 NSERC Alliance Grants (w/Dr. Hongbo Zeng, Qingxia Liu, \$360,000, Co-PI)
Title: *Understanding nucleation, growth, precipitation and breakup behaviors and surface interaction mechanisms of calcite for developing effective anti-scaling strategies in coal mining*
- 07/01/2018 – 12/31/2019 Future Energy Systems (\$30,000, PI)
Title: *CO₂ Adsorption Mechanism of Potassium Promoted Hydrotalcite and its Application in High Purity Hydrogen Production*
- 04/01/2017 – 03/31/2022 NSERC Discovery Grant (\$140,000, PI)
Title: *The Role of Cooperative Atomic Motion in the Plastic Deformation of Metallic Glasses*
- 04/01/2017 – 03/31/2020 Discovery Grants Program – Accelerator Supplements (\$120,000, PI)

- Title: *The Role of Cooperative Atomic Motion in the Plastic Deformation of Metallic Glasses*
- 11/01/2015 – 10/31/2020 NSERC CRD (w/Dr. Weixing Chen, \$1,334,500, Co-PI)
Title: *Predictive crack growth models for pipeline integrity and risk management - phase III*
 - 09/01/2014 – 08/31/2017 C5MPT (w/Dr. Phillip Choi, \$189,000, PI)
Title: *Design of high capacity hydrotalcite for CO₂ capture*
 - 09/01/2014 – 08/31/2017 C5MPT (w/Dr. Hongbo Zeng, Qingxia Liu and Qi Liu, \$300,000, Co-PI)
Title: *Bubble-mineral interaction mechanisms associated with fine particle flotation in complex aqueous media*
 - 04/01/2012 – 03/31/2017 NSERC Discovery Grant (\$120,000, PI)
Title: *Cooperative atomic motion in the interfacial dynamics of strongly interacting particle systems*
 - 07/01/2012 – 06/30/2015 NSERC CRD (w/Dr. Weixing Chen, \$719,330, Co-PI)
Title: *Predictive crack growth models for pipeline integrity and risk management - phase II*
 - 09/01/2007 – 03/31/2012 University Startup Fund (\$100,000, PI)
 - 04/01/2008 – 03/31/2012 NSERC Discovery Grant (\$92,400, PI)
Title: *Deformation mechanisms for nanocrystalline materials in metals*
 - 01/01/2009 – 12/31/2011 NSERC CRD (w/Dr. Weixing Chen, \$789,078, Co-PI)
Title: *Predictive crack growth models for pipeline integrity and risk managements*
 - 01/01/2011 – 08/31/2011 China Opportunity Fund (\$3,850, PI)

SUPERVISED STUDENTS AND POST-DOCS

- 01/01/2023 – present Ms. Yifan Li (Ph.D. student); co-supervised by Dr. Zhi Li
- 09/01/2022 – present Mr. Hanlin Wang (Ph.D. student)
- 09/01/2022 – present Mr. Farhan Khalid (MSc student)
- 01/01/2022 – present Mr. Aliakbar Sheikhzadeh (Ph.D. student)

01/01/2022 – present	Mr. Hongtao Ma (Ph.D. student); co-supervised by Dr. Hongbo Zeng
01/01/2021 – present	Ms. Jiarui Zhang (Ph.D. student)
09/01/2020 – present	Mr. Yue Li (Ph.D. student)
01/01/2019 – 03/24/2023	Ms. Diling Yang (Ph.D. student); Thesis: <i>Probing the Surface Interaction Mechanisms of Air Bubbles and Oil Droplets with Hydrophobic Polymers, Asphaltenes and Bitumen</i>
09/01/2019 – 12/13/2022	Ms. Xuwen Peng (Ph.D. student); co-supervised by Dr. Hongbo Zeng; Thesis: <i>Multifunctional Hydrogels Integrated with Reversible Noncovalent Interactions for Bioengineering and Sensing Applications</i>
09/01/2017 – 09/02/2022	Mr. Gazi Mahmud (Ph.D. student); Thesis: <i>Localization Model Description of Interfacial Dynamics of Free-standing Nanoparticles and Thin Films, and Nanoparticle on Supporting Interacting Substrate</i>
01/01/2019 – 05/06/2022	Ms. Mahsa Nazemi Ashani (MSc student); co-supervised by Dr. Qingxia Liu; Thesis: <i>Atomistic Approach towards Sodium Citrate Role on Surface Properties of Silica and Clay Minerals</i>
09/01/2016 – 12/01/2021	Ms. Xinyi Wang (Ph.D. student); Thesis: <i>Molecular Dynamics Study of Model Systems Showing Dynamic Heterogeneity</i>
09/01/2018 – 08/31/2020	Ms. Haiqing Lu (MEng student); co-supervised by Dr. Qingxia Liu
12/01/2018 – 04/01/2020	Mr. Lintao Gui (Visiting Ph.D. student)
09/01/2016 – 12/05/2020	Mr. Hamid Niazi (Ph.D. student); co-supervised by Dr. Weixing Chen; Thesis: <i>Crack Growth Behaviour of Pipeline Steels under Variable Pressure Fluctuations in a High pH Environment</i>
11/01/2015 – 05/01/2020	Dr. Mohammad Khalkhali (Post-doctoral Fellow); co-supervised by Dr. Qingxia Liu
09/01/2012 – 12/01/2017	Ms. Min Wu (Ph.D. student); co-supervised by Dr. Hongbo Zeng; Thesis: <i>Experimental and Molecular Dynamics Study of the Interactions of Lipid Membranes and the Pulmonary Surfactant-associated Protein B in Model Pulmonary Surfactant Systems</i>

09/01/2015 – 08/31/2017	Mr. Muziyuan Gao (MSc student); Thesis: <i>Study of the thermal stability of hydrotalcite and carbon dioxide capture capacity of hydrotalcite-derived mixed oxides using molecular dynamics simulation</i>
09/01/2012 – 09/30/2016	Mr. Xiao Xing (Ph.D. student); Thesis: <i>Molecular dynamics simulations on crack growth behavior of BCC Fe under variable pressure fluctuations</i>
09/01/2014 – 12/31/2015	Mr. Bin Liu (Visiting Ph.D. student)
01/01/2013 – 11/30/2015	Mr. Xuhang Tong (MSc student); co-supervised by Dr. Dongyang Li; Thesis: <i>The effects of annealing treatment on mechanical properties of nanocrystalline α-iron: an atomistic study</i>
09/01/2011 – 09/30/2015	Ms. Ying Yang (Ph.D. student); Thesis: <i>Effects of size and coalescence on the interfacial dynamics of nanoparticles: a molecular dynamics study</i>
01/01/2011 – 09/30/2015	Mr. Mohammad Khalkhali (Ph.D. Student); co-supervised by Dr. Qingxia Liu; Thesis: <i>On the atomistic simulation approach towards the structural stability of the ZnS nanoparticles</i>
10/01/2012 – 12/31/2012	Mr. Yves Lai (Undergraduate student)
01/09/2012 – 11/30/2012	Mr. Devin Engel (Undergraduate student); co-supervised by Dr. W.X. Chen
09/01/2010 – 11/30/2012	Ms. Di Zhu (MSc student); co-supervised by Dr. Dongyang Li; Thesis: <i>A molecular dynamics simulation study on Bauschinger's effect in nano-scale Cu systems with and without interfaces</i>
04/01/2010 – 03/31/2011	Dr. Xiaoyang Liu (Post-doctoral Fellow); co-supervised by Dr. David Mitlin
01/01/2010 – 12/31/2011	Ms. Arina Marchenko (MSc student); Thesis: <i>A molecular dynamics simulation study on the deformation behavior for nanotwinned polycrystalline copper</i>
09/01/2009 – 09/30/2011	Mr. Wenbo Xie (MSc student); Thesis: <i>Hydrogen induced hardening effects on alpha iron: a molecular dynamics study</i>
04/01/2009 – 03/31/2010	Dr. Xiaoyang Liu (Post-doctoral Fellow)
07/01/2009 – 08/31/2009	Mr. Pranav Kalvapalle (Undergraduate student)
09/01/2007 – 08/31/2009	Mr. Xinan Yan (MSc student); Thesis: <i>Identification of atomistic mechanisms for grain boundary migration</i>

in [001] twist boundaries: molecular dynamics simulation

09/01/2008 – 06/30/2010

Ms. Lei Yue (MSc student); co-supervised by Dr. Dongyang Li; Thesis: *A molecular dynamics modeling study on the mechanical behavior of nano-twinned Cu and relevant issues*

TEACHING EXPERIENCE

Courses Taught

- **MAT E 202, Materials Science II, Department of Chemical and Materials Engineering, University of Alberta:** *An introduction to the science of materials relating their mechanical, thermal, electronic and chemical properties to atomic, molecular and crystal structure. Ceramic and metallic crystals, glasses, polymers and composite materials. Multi-phase materials, strengthening processes. Laboratories include mechanical properties of metals and polymers, microstructure, heat treatment of steel.*
- **MAT E 640, Advanced Materials Thermodynamics, Department of Chemical and Materials Engineering, University of Alberta:** *The aim of this course is to build on thermodynamic principles developed in your undergraduate program. Emphasis will be placed on solutions, phase equilibria in single- and multi-component systems, phase diagrams and reaction equilibria.*
- **MAT E 351, Mechanical Properties, University of Alberta:** *Stress/strain relationships and tensile testing. Dislocation theory, twinning and plastic deformation. Strengthening mechanisms. Fundamentals of fracture, failure mechanisms, fracture mechanics and fracture testing.*
- **CME 483, Colloquium II, Department of Chemical and Materials Engineering, University of Alberta:** *Oral presentation of technical material.*
- **MAT E 694, Computational Materials Science, Department of Chemical and Materials Engineering, University of Alberta:** *The aim of this course is to introduce modern computational material science, i.e., computation and simulation techniques to study materials science, with emphasis on atomistic modeling methodologies and their applications.*
- **Crystallography and Structure of Materials, School of Materials Science and Engineering, University of Science and Technology Beijing:** *An introduction to the science of materials relating their mechanical, thermal, electronic and chemical properties to atomic, molecular and crystal structure.*

- **Computational Materials Science, School of Materials Science and Engineering, University of Science and Technology Beijing:** *An introduction to modern computational material science technologies.*

Instructor Ratings

Course	Year	Class Size	Rating / 5.0
MAT E 202 – Materials Science II	Winter 2008	84	4.0
	Fall 2008	100	3.4
	Fall 2009	104	3.9
	Fall 2010	117	4.4
	Fall 2011	59	4.7
	Fall 2012	115	4.5
	Fall 2014	116	3.9
	Fall 2016	91	4.1
	Fall 2017	91	4.4
	Fall 2018	76	4.1
	Fall 2020	105	3.9
MAT E 640 - Advanced Materials Thermodynamics	Fall 2008	17	3.8
	Fall 2009	38	4.2
	Fall 2010	22	4.3
	Fall 2011	15	4.4
	Fall 2012	29	4.6
	Fall 2014	18	4.0
	Fall 2015	26	4.4
	Fall 2016	30	3.9
	Fall 2017	42	4.6
	Fall 2018	34	4.7
	Fall 2019	33	4.7
	Fall 2020	28	4.4
	Fall 2021	41	4.6
Fall 2022	34	4.7	
MAT E 351 – Mechanical Properties	Winter 2020	21	
CME 483 - Colloquium II	Winter 2013	19	4.2
	Winter 2016	24	4.3
	Winter 2017	25	4.0
CME 481 - Colloquium I	Fall 2017	32	4.6
MAT E 694 – Computational Materials Science	Winter 2015	6	
	Winter 2016	8	

PROFESSIONAL AFFILIATIONS

- Members: The Minerals, Metals & Materials Society (TMS), the Materials Research

Society (MRS), American Society for Engineering Education (ASEE), and the American Physical Society (APS)

SERVICE TO THE DEPARTMENT AND UNIVERSITY

- Associate Dean, Graduate Students (CME) (07/01/2022 – present)
- Associate Chair for Graduate Studies (07/01/2021 – 06/30/2022)
- Canada CIFAR Artificial Intelligence Chair Faculty search committee (03/01/2023 – 06/30/2023)
- Materials Engineering program curriculum review committee
- Masters of Engineering program taskforce
- Mathematics curriculum review committee
- Committee Member, Fraser Russell Teaching Fellowship
- Graduate Advisor for Materials Engineering, Department of Chemical and Materials Engineering (01/01/2012 – present)
- Member, General Faculties Council, University of Alberta, (06/08/2011 – 06/30/2013)
- Vice president, Association of Chinese Canadian Professors (03/01/2010 – 02/01/2014)
- Member, Faculty Search Committee in the Department of Mechanical Engineering (Replacement for Dr. Philip Choi) (01/29/2008)

Examination Committee

- Served in over 200 MSc and PhD examination committee as chair or examiner (09/01/2007 – present)

Committee member for PhD final examination

Ms. Diling Yang Supervisor: Dr. H. Zhang	Mr. Wenshuai Yang Supervisor: Dr. H.B. Zeng	Ms. Ying Wang Supervisor: Dr. P. Mendez
Mr. Bowen Zhang Supervisor: Dr. J.L. Luo	Mr. Pengfei Sui Supervisor: Dr. J.L. Luo	Ms. Lu Sun Supervisor: Dr. H. Henein
Mr. Gazi Mahmud Supervisor: Dr. H. Zhang	Mr. Wensheng Yang Supervisor: Dr. H.B. Zeng	Ms. Xinyi Wang Supervisor: Dr. H. Zhang
Ms. Xuwen Peng Supervisors: H.B. Zeng & H. Zhang	Ms. Qiongyao Peng Supervisor: Dr. H.B. Zeng	Ms. Olayinka Tehinse Supervisor: Dr. W.X. Chen
Mr. Hamid Niazi Supervisor: H. Zhang	Mr. Liam Morrissey Supervisor: S. Nakhla (Memorial University)	Mr. Jeremy Wong Supervisor: Dr. P. Choi
Mr. Wenjihao Hu Superviosr: H.B. Zeng	Mr. Lu Gong Supervisor: Dr. H.B. Zeng	Ms. Hanieh Nassiri Supervisor: Dr. N. Semagina

Mr. Hongbiao Tao Supervisor: Dr. Z.H. Xu	Mr. Nasseh Khodaie Supervisor: Dr. H. Henein	Ms. Zeinab Khorshidi Supervisor: Dr. P. Choi
Ms. Jiawen Zhang Supervisor: Dr. Q.X. Liu	Mr. Linbo Han Supervisor: Dr. H.B. Zeng	Mr. Xin Cui Supervisor: Dr. H.B. Zeng
Mr. Jun Huang Supervisor: Dr. H.B. Zeng	Mr. Fanchao Meng Supervisor: Dr. J. Song (McGill)	Ms. Min Wu Supervisor: Dr. H. Zhang
Mr. Xiao Xing Supervisor: Dr. H. Zhang	Mr. Kaiyang Li Supervisor: Dr. J.L. Luo	Ms. Lin Li Supervisor: Dr. H.B. Zeng
Mr. Yinan Wang Supervisor: Dr. R. Narain	Mr. Yashar Behnamian Supervisor: Dr. J.L. Luo	Mr. Mohammad Khalkahli Supervisor: Dr. H. Zhang
Mr. Syed Jawad Shah Supervisor: Dr. H. Henein	Ms. Ying Yang Supervisor: Dr. H. Zhang	Mr. Peyman Saidi* Supervisor: Dr. J. Hoyt (McMaster)
Mr. Xiaotian Zhang Supervisor: Dr. W.X. Chen	Mr. Mengshan Yu Supervisor: Dr. W.X. Chen	Mr. Xuehai Tan Supervisor: Dr. D. Mitlin
Mr. Abolfazl Noorjahan Supervisor: Dr. P. Choi	Mr. Alireza Kohandehghan Supervisor: Dr. D. Mitlin	Ms. Leylisadat Mirmontazeri Supervisor: Dr. A. Yeung
Ms. Elmira Memarzadehlotfabad Supervisor: Dr. D. Mitlin	Mr. Ali Faghihnejad Supervisor: Dr. H.B. Zeng	Mr. Kazi Md Shammi Tunvir Supervisor: Dr. C.Q. Ru
Mr. Zhiqiang Dong Supervisor: Dr. W.X. Chen	Mr. Benjamin Zahiri Supervisor: Dr. D. Mitlin	Mr. Mohammad Chowdhuri Supervisor: Dr. Z.H. Xia
Mr. Eric Luber Supervisor: Dr. D. Mitlin	Mr. Mohsen Danaie Supervisor: Dr. D. Mitlin	Mr. Colin Ophus Supervisor: Dr. D. Mitlin

SERVICE TO THE COMMUNITY

- Editorial Board Member for Journal of Pipeline Science and Engineering (01/01/2021 – present)
- Editorial Board Member for Scientific Reports (09/2016 – present)
- Member of APEGA Board of Examiners (08/2016 – present)
- Organizer, Multiscale Modelling and Simulations of Failure in Structural Materials, COM 2014, October, 2014
- Invited speaker, ENGG 101, Orientation to the Engineering Profession II, Grant MacEwan University (01/25/2013)
- Invited speaker, ENGG 101, Orientation to the Engineering Profession II, Grant MacEwan University (01/27/2012)
- Session Chair, Deformation and Transitions at Grain Boundaries, Materials Science & Technology 2011, Columbus (10/16/2011 – 10/20/2011)
- Session Chair, Computational Science of Transport Phenomena in Materials: Methods and Applications, International Conference on Materials for Advanced Technologies,

Singapore, (06/26/2011 – 07/01/2011)

- Organizer, 20th Canadian Materials Science Conference, Edmonton (06/2008)
- Key Reader, Metallurgical and Materials Transactions A (03/01/2008 – present)

PEER-REVIEW ACTIVITIES

Peer-reviewed Journals

<i>ACS Nano</i>	<i>ACS Sustainable Chemistry & Engineering</i>	<i>Acta Materialia</i>
<i>Acta Metallurgica Sinica</i>	<i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i>	<i>Advanced Engineering Materials</i>
<i>Advanced Functional Materials</i>	<i>Advanced Materials</i>	<i>Advanced Materials Interfaces</i>
<i>Applied Optics</i>	<i>Applied Surface Science</i>	<i>Advanced Theory and Simulations</i>
<i>Canadian Journal of Physics</i>	<i>Carbon</i>	<i>Chemistry of Materials</i>
<i>Composite Interfaces</i>	<i>Computational Materials</i>	<i>Computational Materials Science</i>
<i>Computer Physics Communications</i>	<i>Corrosion Science</i>	<i>Energy & Fuels</i>
<i>Engineering Failure Analysis</i>	<i>Engineering Fracture Mechanics</i>	<i>Environmental Science & Technology</i>
<i>Industrial & Engineering Chemistry Research</i>	<i>Intermetallics</i>	<i>International Journal of Hydrogen Energy</i>
<i>International Journal of Nano and Biomaterials</i>	<i>Journal of Alloys and Compounds</i>	<i>Journal of Applied Physics</i>
<i>Journal of Advanced Dielectrics</i>	<i>Journal of Chemical Physics</i>	<i>Journal of CO₂ Utilization</i>
<i>Journal of Materials Research</i>	<i>Journal of Materials Science</i>	<i>Journal of Materials Science & Technology</i>
<i>Journal of Molecular Liquids</i>	<i>Journal of Nanomaterials</i>	<i>Journal of Physical Chemistry</i>
<i>Journal of Physical Chemistry Letters</i>	<i>Journal of Physics and Chemistry of Solids</i>	<i>Journal of Physics: Condensed Matter</i>
<i>Journal of Strain Analysis for Engineering Design</i>	<i>Materials Chemistry and Physics</i>	<i>Materials Today</i>
<i>Materials Today Communications</i>	<i>Materials Science and Technology</i>	<i>Macromolecules</i>
<i>Metallurgical and Materials Transactions A</i>	<i>Modelling and Simulation in Materials Science and Engineering</i>	<i>Modern Physics Letters B</i>
<i>Nanoscale</i>	<i>Nature Communications</i>	<i>Optics Express</i>
<i>Philosophical Magazine Letters</i>	<i>Physica Status Solidi (b)</i>	<i>Polymer Chemistry</i>
<i>Physical Chemistry Chemical Physics</i>	<i>Proceedings of the National Academy of Sciences of the United States of America</i>	<i>RSC Advances</i>
<i>Science Advances</i>	<i>Scientific Reports</i>	<i>Scripta Materialia</i>

<i>Separation and Purification Technology</i>	<i>Small</i>	<i>Soft Matter</i>
<i>Solid State Communications</i>		

Grants

<i>CFI Leaders Opportunity Fund</i>	<i>DOE Office of Basic Energy Sciences</i>	<i>Ontario Centres of Excellence</i>
<i>New Researchers Start-up Program (Quebec)</i>	<i>NSERC Canada Research Chair</i>	<i>NSERC Discovery Grant</i>
<i>NSERC Strategic Grant</i>	<i>Israel Science Foundation</i>	<i>SSHRC New Frontiers in Research Fund</i>

PUBLICATIONS (students' names are boldfaced; star indicates corresponding authors)

Refereed Papers

1. X.L. Gao, **Y. Li**, H.X. Li, X.Z. Zhang, Z.Q. Zhang, H. Zhang, G. Li*, *Surface-induced Co/Co₉S₈ nanodots embedded in nitrogen-doped hollow carbon nanocubes for high-performance overall water splitting*, ***Sustainable Materials and Technologies***, in press; (2023)
2. **D.L. Yang**, C.Y. Qiao, X.H. Mao, J.Y. Wang, L. Xie, J.S. Chen, **X.W. Peng**, Q.Y. Peng, T. Wang, Q. Liu, H. Zhang*, H.B. Zeng*, *Probing the surface forces between air bubbles and bitumen via direct force measurements: effects of aqueous chemistry*, ***Fuel***, 357, 129865; (2024)
3. H.F. Sun, M.F. Li, H. Zhang, J. Liu*, *Phase transformation and diffusion in high-temperature oxidation of FeCrNi medium entropy alloy*, ***Corrosion Science***, 227, 111685; (2024)
4. O.B. Wani, **D.L. Yang**, S. Manzoor, M. Shoaib, S. Khan, H. Zhang, H.B. Zeng, B. Klein, E. Bobicki*, *Modulating particle-particle interaction in Phyllosilicate Serpentine aqueous suspensions using Sodium Citrate*, ***Journal of Environmental Chemical Engineering***, 11, 111213; (2023)
5. G.C. Lv, W.J. Qian, H. Zhang, Y. Su, P. Qian*, *Role of -O functional groups at the Ti₃C₂O₂(MXene)/Al interface in enhancing the mechanical properties of aluminum matrix composites: A first-principles study*, ***Applied Surface Science***, 642, 158608; (2023)
6. Y. Dong, S. Liu, W.J. Deng, H. Zhang, G.Y. Liu, X.L. Wang*, *Modulating electronic structures of bimetallic Co-Fe sulfide ultrathin nanosheet supported on g-C₃N₄ for highly electrocatalytic hydrogen evolution performance*, ***Journal of Colloid and Interface***

- Science**, 653, 1557-1565; (2023)
7. Y. Dong, Z.P. Deng, H. Zhang, G.Y. Liu, X.L. Wang*, *A highly active and durable hierarchical electrocatalyst for large-current-density water splitting*, **Nano Letters**, 23, 9087-9095; (2023)
 8. L.Y. Zhu, W.S. Lyu, X.H. Mao, Z.Q. Zhao, **D.L. Yang**, H. Zhang, K. Wang, P. Yang*, H.B. Zeng*, *Effect of solution pH and polyethylene oxide concentration on surface/interface properties, flocculation and rheology of concentrated monodisperse ultrafine tailings slurry*, **Powder Technology**, 430, 119002; (2023)
 9. B.L. Xiang, **M.N. Ashani**, Z.Q. Zhang, R. Manica, H. Zhang, Q.X. Liu*, *Competitive adsorption between sodium citrate and naphthenic acids on alumina surfaces: Experimental and computational study*, **Minerals Engineering**, 203, 108324; (2023)
 10. **Y. Li**, H.B. Zeng, H. Zhang*, *Atomistic simulations of nucleation and growth of CaCO₃ with the influence of inhibitors: A review*, **Materials Genome Engineering Advances**, e4; (2023)
 11. **Y. Li**, H.B. Zeng, H. Zhang*, *Influence of impurity metal doping on calcite growth: a first-principles study*, **Applied Surface Science**, 637, 157927; (2023)
 12. Z.X. Xu, **Y. Li**, G. Li, H. Zhang*, X.L. Wang*, *Reversible zinc powder anode via crystal facet engineering*, **Matter**, 6, 3075-3086; (2023)
 13. H. Zhang*, **X.Y. Wang**, **J.R. Zhang**, H.B. Yu, J.F. Douglas*, *Approach to hyperuniformity in a metallic glass-forming material exhibiting a fragile to strong glass transition*, **The European Physical Journal E**, 46, 50; (2023)
 14. **D.L. Yang**, Z.Q. Zhao, L. Gong, Y.X. Sun, X.W. Peng, Q.Y. Peng, T. Wang, Q. Liu, H. Zhang*, H.B. Zeng*, *Surface interaction mechanisms of air bubbles, asphaltenes and oil drops in aqueous solutions with implications for interfacial engineering processes*, **Journal of Colloid and Interface Science**, 647, 264-276; (2023)
 15. Q. Sun, J.S. Chen, Z.Q. Zhao, **D.L. Yang**, Y.Y. Xiao, H. Zhang, X. Ma, H. Zhong, H.B. Zeng*, *Tailored pH-triggered surfactant for stepwise separation of a three-component mineral system*, **Separation and Purification Technology**, 316, 123753; (2023)
 16. **X.W. Peng**, Q. Peng, M. Wu, W.D. Wang, Y.F. Gao, X. Liu, Y.X. Sun, **D.L. Yang**, Q.Y. Peng, T. Wang, X.Z. Chen, J.F. Liu*, H. Zhang*, H.B. Zeng*, *A pH and temperature dual-responsive microgel-embedded, adhesive and tough hydrogel for drug delivery and wound healing*, **ACS Applied Materials & Interfaces**, 15, 19560-19573; (2023)
 17. Y.M. Chen, F.C. Gong, W.J. Deng, H. Zhang, X.L. Wang*, *Dual-function electrolyte additive enabling simultaneous electrode interface and coordination environment*

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133. **L. Yue**, H. Zhang, D.Y. Li*, *Defect generation in nano-twinned, nano-grained and single-crystal Cu systems caused by wear - a molecular dynamics study*, **Scripta Materialia**, 63: 1116-1119; (2010).
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142. H. Zhang*, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Characterization of atomic motions governing grain boundary migration*, **Physical Review B**, 74: 115404; 2006; also selected in **Virtual Journal of Nanoscale Science and Technology**, 14: 13; (2006).
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148. M.I. Mendeleev, H. Zhang* and D.J. Srolovitz, *Grain boundary self-diffusion in Ni: effect of boundary inclination*, **Journal of Materials Research**, 20: 1146-1153; (2005).
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150. H. Zhang*, M.I. Mendeleev, D.J. Srolovitz, *Computer simulation of the elastically-driven migration of a flat grain boundary*, **Acta Materialia**, 52: 2569-2576; (2004).
151. H. Zhang, Z.N. Xia*, *Molecular dynamics simulation of cluster beam Al depositing on Si (100) substrate*, **Nuclear Instruments & Methods in Physics Research Section B - Beam Interactions with Materials and Atoms**, 160: 372-376; (2000).
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Book Chapters

153. H. Zhang, J.F. Douglas, *Similarities of the Collective Interfacial Dynamics of Grain*

*Boundaries and Nanoparticles to Glass-Forming Liquids; **Advances in Chemical Physics**, Vol. 152, Liquid Polymorphism, H.E. Stanley, March (2013).*

Peer-reviewed Conference Papers

154. **H. Niazi**, H. Zhang*, L. Lamborn, W.X. Chen, The impact of pressure fluctuations on the early onset of stage II growth of high pH stress corrosion crack, ***Proceedings of 13th International Pipeline Conference***, IPC2020-9511, 1-11; (2020)
155. **H. Niazi**, H. Zhang*, K. Korol, W.X. Chen, *High pH crack growth sensitivity to underload-type of pressure fluctuations*, ***Proceedings of 12th International Pipeline Conference***, IPC2018-78394, 1-8; (2018)
156. **X. Xing**, M.S. Yu, O. Tehinse, W.X. Chen, H. Zhang*, *The effects of pressure fluctuations on hydrogen embrittlement in pipeline*, ***Proceedings of 11th International Pipeline Conference***, IPC2016-64478, 1-10; (2016).

PRESENTATIONS (underline indicates presenter)

Invited Talks

1. *Adsorption and dissociation of hydrogen on pipeline steel under supercritical conditions, China University of Petroleum, Qingdao, China, November, 2023*
2. *Adsorption and dissociation of hydrogen on iron and iron oxide surfaces under supercritical conditions, University of Science and Technology Beijing, China, July, 2023*
3. *Understanding hydrogen effect in pipeline steels from atomistic perspective, China International Pipeline Conference, China, April, 2023 (Virtual)*
4. *The role of collective atomic motion in hierarchical relaxations in metallic glasses, Symposium of Amorphous and High Entropy Alloys, Hangzhou, China, November, 2022 (Virtual)*
5. *Dynamic heterogeneity in metallic glass-forming alloys – A perspective from local caged atomic motion, 33rd Canadian Materials Science Conference, June, 2022*
6. *Computational Materials Science and its Application on CO₂ Capture using Solid Sorbents, Tiangong University, China, November, 2019*
7. *Molecular dynamics simulation of structure evolution of hydrotalcite and CO₂*

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- adsorption behavior in hydrotalcite and its derived oxides, 31th Canadian Materials Science Conference, June, 2019*
8. *Computational Materials Science and its Application in Hydrogen Embrittlement in Pipeline Steel, University of Science and Technology Beijing, April, 2019*
 9. *Mechanical Behavior of Nanostructured Materials: Molecular Dynamics Studies, Beijing University of Technology, April, 2019*
 10. *Computational Materials Science and its Application in Structure Characterization of Hydrotalcite, Beijing University of Chemical Technology, April, 2019*
 11. *Computational Materials Science and its Application in Hydrogen Embrittlement in Steels, Nanjing Tech University, April, 2019*
 12. *The role of collective atomic motions on interface diffusion, relaxation, and migration, Southern University of Science and Technology, October, 2018*
 13. *Computational Materials Science and its Application in Pipeline Steels, China University of Petroleum, July, 2018*
 14. *The Role of Collective Atomic Motions on Interface Relaxation, Migration and Deformation, University of Manitoba, August, 2018*
 15. *Unified Way to Characterize Locally Close-Packed Particles in Metallic Glass Systems, Zhejiang University, June, 2018*
 16. *The Role of Collective Atomic Motions on Interface Migration and Deformation, TMS 2017, February, 2017*
 17. *Atomistic Simulations on the Structural Stability of the ZnS Nanoparticles in Bare and Hydrated States, Zhejiang University, April, 2017*
 18. *Localization Model Description of Diffusion and Structural Relaxation in Cu-Zr Metallic Glasses, Zhejiang University, April, 2016*
 19. *Effects of Annealing on Mechanical Properties of Nanocrystalline α -iron, MS&T 2015, October, 2015*

20. *String-like Cooperative Motion in Supercooled Cu-Zr Metallic liquids*, 2nd International Workshop on Challenges of Atomistic Computer Simulations of Glass and Amorphous Materials, June, 2015
21. *String-like Cooperative Motion in Supercooled Cu-Zr Metallic liquids*, Zhejiang University, June, 2015
22. *Effects of Nano-scale Grain Boundaries and Twin Boundaries in Cu on its Bauschinger's Effect and Response to Cyclic Deformation*, COM 2014, September, 2014
23. *Understanding Structure-Property Relationship at the Atomic Level*, School of Chemistry and Chemical Engineering, Central South University, April, 2014
24. *Mechanical Behavior in Nanostructured Materials: Molecular Dynamics Studies*, School of Aerospace Engineering, Tsinghua University, November, 2013
25. *Mechanical Response in Nanostructured Materials: Molecular Dynamics Studies*, Department of Engineering Mechanics, Xi'an Jiaotong University, October, 2013
26. *Hydrogen Diffusion, Hardening and H-induced Phase Transformation in α -iron: Molecular Dynamics Simulations*, 2013 China Environmental Fracture Conference, Wuyuan, October, 2013
27. *Hydrogen Diffusion and Hardening in α -iron: Molecular Dynamics Simulations*, McMaster University, Hamilton, November, 2012
28. *Collective Atomic Motion in the Strongly Interacting Particle Systems*, National Institute of Standards and Technology, Maryland, August, 2012
29. *Cooperative Atomic Motion in the Strongly Interacting Particle Systems*, Wuhan University of Technology, Wuhan, May, 2012
30. *Grain Boundary Sliding in FCC and HCP Metals*, Materials Science & Technology 2011, Columbus, October, 2011
31. *Molecular Dynamics Simulation of Mechanical Response in Nanostructured Cu*, International Congress on Industrial and Applied Mathematics, Vancouver, July, 2011
32. *Cooperative Atomic Motions in the Interfacial Dynamics of Nanoparticles*, International

Conference on Materials for Advanced Technologies, Singapore, June, 2011

33. *String-like Cooperative Motions in the Interfacial Dynamics of Nanoparticles*, University of Shanghai for Science and Technology, Shanghai, May, 2011
34. *String-like Cooperative Motions in the Interfacial Dynamics of Nanoparticles*, Northwestern Polytechnical University, Xi'an, April, 2011
35. *String-like Cooperative Motions during Grain Boundary Migration*, Xi'an Jiaotong University, Xi'an, April, 2011
36. *Atomistic Simulation of Grain Boundary Migration*, Institute of Metal Research, Shenyang, April, 2011
37. *Grain Boundaries and Glasses: Birds of a Feather*, Department of Materials Science and Engineering, Tsinghua University, Beijing, December, 2010
38. *Grain Boundary Sliding in Mg: A Molecular Dynamics Study*, MagNET Workshop V, Vancouver, October, 2010
39. *Mechanical Response in Nanocrystalline Aluminum at High Temperature and Strain Rate*, 9th World Congress on Computational Mechanics and 4th Asian Pacific Congress on Computational Mechanics, Sydney, July, 2010
40. *Grain Boundary Migration in Mo and Mo-Ni Alloy*, Bridging the Gap Workshop, Department of Materials Science and Engineering, McMaster University, Hamilton, October, 2009
41. *How Do Atoms Move during Grain Boundary Migration?* Advanced Materials and Process Engineering Laboratory, University of British Columbia, Vancouver, February, 2008
42. *Atomistic Mechanisms for Grain Boundary Migration*, Department of Materials Science, University of Science and Technology Beijing, Beijing, July, 2008
43. *Overview of Molecular Dynamics Simulations of Grain Boundary Migration*, School of Materials Science and Engineering, Shanghai Jiaotong University, Shanghai, December, 2007

44. *Grain Boundary Migration: Molecular Dynamics Studies*, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, December, 2007

Contributed Talks and Presentations

45. H. Zhang, Molecular dynamics simulation of CO₂ adsorption behavior in hydrotalcite and its derived oxides, TMS 2020, San Diego, USA, February, 2020

46. H. Niazi, W.X. Chen, H. Zhang, Effects of stress intensity factor and loading spectra on intergranular SCC crack growth, 31th Canadian Materials Science Conference, June, 2019

47. H. Niazi, H. Zhang, Influence of underload cycle on crack growth behavior of X65 pipeline steel in carbonate/bicarbonate environment, 30th Canadian Materials Science Conference, June, 2018

48. G. Mahmud, H. Zhang, Molecular Dynamics Study of Dynamic Properties of Cu₆₄Zr₃₆ Metallic Glass Nanoparticles, 30th Canadian Materials Science Conference, June, 2018

49. X.Y. Wang, H. Zhang, Molecular dynamics simulation on the interfacial dynamics of ice, 30th Canadian Materials Science Conference, June, 2018

50. M.Z.Y. Gao, H. Zhang, *Molecular Dynamics Simulations of Thermal Stability and Capacity of Carbon Dioxide Capture in Hydrotalcite*, 29th Canadian Materials Science Conference, June, 2017

51. H. Zhang, *String-like Cooperative Motion in Supercooled Cu-Zr Metallic Liquids*, TMS 2016, February, 2016

52. X. Xing, W.X. Chen, H. Zhang, *Prediction of Crack Propagation in Pipeline Steel under Cyclic Loading Condition*, MS&T 2015, October, 2015

53. X.H. Tong, H. Zhang, D.Y. Li, *Effect of Annealing Treatment on Mechanical Properties of Nanocrystalline α -iron: an Atomistic Study*, COM 2014, September, 2014

54. Hao Zhang, *Molecular Dynamics Simulation of Effect of Hydrogen at Crack Tip in Fe*, SINOCORR 2014, May, 2014

55. Hao Zhang, *Colored Noise, Dynamic Heterogeneity and Collective Atomic Motion in the Interfacial Dynamics of Ni Nanoparticles*, China Nano, September, 2013

56. D. Zhu, H. Zhang, D.Y. Li, *Influence of Twin-Boundary on the Bauschinger's Effect in Cu Crystal- A Molecular Dynamics Simulation Study*, TMS Annual Meeting, Orlando, March, 2012
57. A. Marchenko, H. Zhang, *The Effect of Twin Spacing and Grain Size on the Plastic Deformation of Nanocrystalline Copper*, Materials Science & Technology 2011, Columbus, October, 2011
58. W.B. Xie, W.X. Chen, H. Zhang, *Hydrogen Hardening Effect in Heavily Deformed Single Crystal alpha-iron*, Materials Science & Technology 2011, Columbus, October, 2011
59. A. Marchenko, H. Zhang, *Effects of Twin Spacing on Plastic Deformation of Nanocrystalline Copper*, Faculty of Engineering Graduate Research Symposium, Edmonton, June, 2011
60. W.B. Xie, W.X. Chen, H. Zhang, *Hydrogen Effects in Heavily Deformed Nano-Structured Alpha Iron: Molecular Dynamics Study*, Faculty of Engineering Graduate Research Symposium, Edmonton, June, 2011
61. H. Zhang, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Grain Boundaries and Glasses: Birds of a Feather*, APS Annual Meeting, Portland, Oregon, March, 2010
62. H. Zhang, X.N. Yan, *Molecular Dynamics Simulations of Atomistic Mechanisms for Grain Boundary Migration in [001] Twist Boundaries*, TMS Annual Meeting, Seattle, February, 2010
63. H. Zhang, *Atomistic Simulation of Grain Boundary Sliding in Mg during High Temperature Deformation*, TMS Annual Meeting, Seattle, February, 2010
64. L. Yue, D.Y. Li, H. Zhang, *Responses of Twin and Grain Boundaries at Nanometer Scale to Mechanical Attacks - A Molecular Dynamics Simulation Study*, MRS Fall Meeting, Boston, December, 2009
65. X.N. Yan, H. Zhang, *Atomistic Mechanisms for Grain Boundary Migration in [001] Twist Boundaries*, Graduate Research Symposium, Edmonton, May, 2009
66. X.N. Yan, H. Zhang, *Grain Boundary Migration in $\Sigma 5$ [001] Twist Boundary: Molecular Dynamics Study*, 20th Canadian Materials Science Conference, Edmonton, June, 2008

67. H. Zhang, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Statistical Characterization of Atomistic Motion during Grain Boundary Migration*, TMS Annual Meeting, Orlando, February, 2007
68. H. Zhang, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Glass-like Behavior in General Grain Boundary During Migration*, Fourteenth Computational Materials Science Network Workshop, Yeshiva University, NY, February, 2007
69. H. Zhang, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Atomistic Mechanism for Grain Boundary Migration: Molecular Dynamics Studies*, Gordon Research Conference on Physical Metallurgy, New Hampshire, July, 2006 (Poster Presentation)
70. H. Zhang, D.J. Srolovitz, J.F. Douglas, J.A. Warren, *Characterization of Atomic Motions Governing Grain Boundary Dynamics*, Thirteenth Computational Materials Science Network Workshop, Lake Tahoe, April, 2006
71. H. Zhang, D.X. Du, D.J. Srolovitz, *Shear Induced Grain Boundary Migration: A Mechanistic Study*, Thirteenth Computational Materials Science Network Workshop, Lake Tahoe, April, 2006
72. H. Zhang, D.J. Srolovitz, *Grain Boundary Migration Mechanism: $\Sigma 5$ Tilt Boundaries*, Eleventh Computational Materials Science Network Workshop, Northeastern University, Boston, May, 2005
73. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *Dependence of Grain Boundary Mobility on Boundary Plane*, TMS Annual Meeting, San Francisco, February, 2005
74. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *Determination of Grain Boundary Stiffness*, Tenth Computational Materials Science Network Workshop, Northwestern University, Chicago, October, 2004
75. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *Stress-driven Grain Boundary Migration: Effect of Boundary Inclination on Mobility*, TMS Annual Meeting, Charlotte, March, 2004
76. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *The Effect of Inclination on Grain Boundary Mobility*, Ninth Computational Materials Science Network Workshop, ORNL, March, 2004
77. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *Molecular Dynamics Simulation of Stress*

Induced Grain Boundary Migration in Nickel, MRS Fall Meeting, Boston, December, 2003 (Poster Presentation)

78. H. Zhang, M.I. Mendeleev, D.J. Srolovitz, *Stress Driven Migration of Flat Grain Boundaries*, Eighth Computational Materials Science Network Workshop, Colorado School of Mines, October, 2003
79. H. Zhang, D.J. Srolovitz, *Molecular Dynamics Simulation of Grain Boundary Migration in Three Dimension*, Gordon Research Conference on Physical Metallurgy, New Hampshire, July, 2002 (Poster Presentation)
80. H. Zhang, D.J. Srolovitz, *Temperature Dependence of Grain Boundary Migration in 3-D*, Fifth Computational Materials Science Network Workshop, NIST, March, 2002