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Dr. Chandra Veer Singh

Correspondence language: English

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Dr. Chandra Veer Singh

Language Skills

Language	Read	Write	Speak	Understand	Peer Review
English	Yes	Yes	Yes	Yes	Yes
Hindi	Yes	Yes	Yes	Yes	No

Degrees

- 2008/12 Doctorate, Aerospace Engineering, Texas A & M University
Supervisors: Talreja, R., 2005/9 - 2008/12
- 2003/1 Master's Thesis, Satellite Technology and Applications, Indian Institute of Science
Supervisors: Dattaguru, B., 2001/7 - 2003/1
- 2001/6 Bachelor's, Mechanical Engineering, Dayalbagh Educational Institute, India
Supervisors: Hans Raj, K., 1997/7 - 2001/6

Recognitions

- 2018/4 - 2021/3 NSERC Discovery Accelerator Supplement (DAS) - 120,000
Natural Sciences and Engineering Research Council of Canada (NSERC)
Prize / Award
The DAS Program provides substantial and timely resources to researchers who have a superior research program that is highly rated in terms of originality and innovation, and who show strong potential to become international leaders within their field.
- 2017/7 - 2019/4 Connaught Global Challenge Award - 1,000,000
Connaught Fund
Prize / Award
\$1M team award for a multidisciplinary team of leading UofT researchers to enhance UofT's capacity to develop solutions to important global issues facing society. Our Solar Fuels cluster is led by G.A. Ozin of Chemistry.
- 2017/4 - 2022/3 Ontario Early Researcher Award - 190,000
Government of Ontario
Prize / Award
Awarded to promising, recently-appointed Ontario researchers to help build their research teams and helps Ontario's ability to attract and retain the best and brightest research talent. Five year term.

2017/1 - 2021/6 Erwin Edward Hart Endowed Professorship in Materials Science & Engineering - 225,000
Hart Foundation
Prize / Award
These inaugural professorships are awarded to seven professors within the Faculty of Applied Science & Engineering at the University of Toronto who are within the first 10 years of their careers and have demonstrated a high level of research excellence and exemplary graduate student mentorship. Three year term.

User Profile

Research Specialization Keywords: Computational Materials Science, Materials Science & Technology, Materials for Sustainable Energy, Composite Materials, Damage and Failure of Engineering Materials, Nanomaterials

Employment

2022/7 Professor
Materials Science and Engineering, University of Toronto
Full-time, Professor
Tenure Status: Tenure

2017/7 Associate Chair of Research
Materials Science and Engineering, St. George, University of Toronto
Full-time, Professor
Tenure Status: Tenure
Associate Chair for Research and Partnerships for the department

2023/7 - 2023/8 Acting Chair
Materials Science and Engineering, University of Toronto
Full-time, Professor
Tenure Status: Tenure
Acting chair of the department

2021/1 - 2023/6 Associate Director of Academic Programs
Acceleration Consortium, St. George, University of Toronto
Full-time, Professor
Tenure Status: Tenure
Associate Director of Academic Programs for the Acceleration Consortium at UofT

2016/7 - 2022/6 Associate Professor
Materials Science and Engineering, St. George, University of Toronto
Full-time, Associate Professor
Tenure Status: Tenure

2016/7 - 2021/6 Erwin Edward Hart Endowed Professor
Materials Science and Engineering, St. George, University of Toronto
Full-time, Associate Professor
Tenure Status: Tenure

2017/8 - 2018/8 Engineering Fellow
Integran Technologies
On research leave (sabbatical)

2011/9 - 2016/6 Assistant Professor
Materials Science & Engineering, Faculty of Applied Science & Engineering, University of Toronto
Full-time, Assistant Professor
Tenure Status: Tenure Track

2009/1 - 2011/9	Postdoctoral Associate Faculty of Engineering, Cornell University Ithaca, New York, USA.
2005/8 - 2008/12	Graduate Research Assistant Texas A & M University College Station, Texas, USA.
2003/2 - 2005/8	Design Engineer Aircraft Engines, General Electric (GE) Aviation Bangalore, India.
2001/7 - 2003/1	Project Associate Satellite Technology Lab, Indian Institute of Science Bangalore, India
2000/5 - 2000/7	Summer Intern Aerial Delivery Research and Development Establishment (ADRDE) Agra, India.
1999/5 - 1999/7	Summer Intern Bharat Heavy Electricals Ltd. (BHEL) Hardwar, India.

Leaves of Absence and Impact on Research

2017/7 - 2018/8	Sabbatical, University of Toronto Research leave to initiate collaborations with industry: Tata Research Development and Design Centre (India) and Integran Technologies (Canada). During this visit, I saw first-hand how materials science industry is changing. This helped me initiate two new research directions in my group on additive manufacturing and AI; leading to practically impactful work and enhancing research productivity. Impact: positive. New research directions started.
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Research Funding History

Awarded [n=10]

2023/4 - 2029/3 Co-applicant	CANSTOREnergy: Seasonal storage of renewable energy, Grant Funding Sources: New Frontiers in Research Fund - Transformation Transformation Total Funding - 24,000,000 Portion of Funding Received - 1,000,000 Funding Competitive?: Yes
2023/4 - 2028/3 Co-applicant	Toronto Integrated Platform for Materials under Extreme Conditions (TIME), Grant Funding Sources: Canada Foundation for Innovation (CFI) Infrastructure fund Total Funding - 7,247,506 Portion of Funding Received - 724,750 Funding Competitive?: Yes Co-applicant : Yu Zou

2023/4 - 2026/3 Co-applicant	<p>Autonomous Adaptive Design & Discovery of Novel High Entropy Oxide Oxygen Evolution Reaction (HEROIC) Catalysts, Grant</p> <p>Funding Sources: National Research Council Canada (NRC) (Ottawa, ON) Collaborative Research Grant Total Funding - 912,813 Portion of Funding Received - 456,406 Funding Competitive?: Yes</p>
2011/9 - 2025/6 Co-investigator	<p>Start-up Grant for Computational Materials Engineering Laboratory, Grant</p> <p>Funding Sources: University of Toronto University Startup Fund Total Funding - 160,000 Portion of Funding Received - 95,000 Funding Competitive?: No</p>
2017/10 - 2024/9 Co-investigator	<p>Design, Manufacturing and Process Integration of Nano-structured Carbon Enhanced Lightweight Composites, Grant</p> <p>Funding Sources: Hutchinson Aerospace & Industry - Montreal Total Funding - 250,000 Portion of Funding Received - 0 Funding Competitive?: Yes Ford Motor Company - Windsor Total Funding - 750,000 Portion of Funding Received - 0 Funding Competitive?: Yes Natural Sciences and Engineering Research Council of Canada (NSERC) CRD Total Funding - 2,000,000 Portion of Funding Received - 140,000 Funding Competitive?: Yes</p> <p>Principal Applicant : Sain, M.</p>
2022/8 - 2024/7 Principal Applicant	<p>Establishing an experimental and theoretical basis for 2D Polymers for CO₂ Conversion, Grant</p> <p>Funding Sources: University of Toronto Xseed collaborative grant Total Funding - 120,000 Portion of Funding Received - 60,000 Funding Competitive?: Yes</p> <p>Co-applicant : Dwight Seferos</p>
2019/7 - 2024/6 Principal Applicant	<p>Towards U of T Centre on 2D Materials, with Application to Infrastructure, Aerospace, Transportation, and Energy Technologies, Grant</p> <p>Funding Sources: University of Toronto Faculty of Applied Sci & Eng - Dean's strategic grant Total Funding - 420,000 Portion of Funding Received - 140,000 Funding Competitive?: Yes</p>

2021/3 - 2024/3 Principal Applicant	Accelerating Design & Development of High Entropy Alloys using Machine Learning, Contract Funding Sources: National Research Council Canada (NRC) (Ottawa, ON) AI for Materials Design Total Funding - 280,000 Portion of Funding Received - 280,000 Funding Competitive?: Yes
2018/4 - 2024/3 Principal Applicant	Probabilistic Machine Learning Driven Discovery and Design of New Materials for Sustainable Energy and Transport, Grant Funding Sources: Natural Sciences and Engineering Research Council of Canada (NSERC) Discovery Total Funding - 384,000 Portion of Funding Received - 384,000 Funding Competitive?: Yes
2020/4 - 2023/6 Principal Applicant	AI driven design and development of all solid state electrolytes for consumer electronics, Contract Funding Sources: National Research Council Canada (NRC) (Ottawa, ON) Collaboration Centre in Green Energy Materials (CC-GEM) Total Funding - 85,000 Portion of Funding Received - 85,000 Funding Competitive?: Yes
Completed [n=22]	
2020/7 - 2022/6 Co-applicant	Dense, Metal-rich Diamondoid Materials: Computational Materials Engineering and Chemical Synthesis Join Forces, Grant Funding Sources: University of Toronto Xseed grant Total Funding - 120,000 Portion of Funding Received - 60,000 Funding Competitive?: Yes
2016/7 - 2022/6 Co-investigator	Toward a Centre in Computational Science & Engineering, Grant Funding Sources: University of Toronto Dean's Strategic Fund Total Funding - 181,000 Portion of Funding Received - 18,000 Funding Competitive?: Yes Principal Investigator : David Zingg
2016/4 - 2022/3 Principal Investigator	Integrated Computational Materials Engineering of Ultra-lightweight Alloys with Unprecedented Ductility and Mechanical Strength for Automotive and Aerospace applications, Grant Funding Sources: Ontario Ministry of Research and Innovation (ON) Early Researcher Award Total Funding - 140,000

Portion of Funding Received - 140,000
 Funding Competitive?: Yes
 University of Toronto
 Total Funding - 50,000
 Portion of Funding Received - 50,000
 Funding Competitive?: Yes
 Collaborator : Integran Technologies

2020/4 - 2022/3
 Principal Applicant

AI Driven Design and Optimization of Surface Adsorbents for Removal of Contaminant Minerals from Contaminated Water, Grant

Funding Sources:

University of Toronto
 Waterseed grant (internal)
 Total Funding - 120,000
 Portion of Funding Received - 60,000
 Funding Competitive?: Yes

2018/4 - 2022/3
 Principal Applicant

Probabilistic Machine Learning Driven Discovery and Design of New Materials for Sustainable Energy and Transport, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
 Discovery Accelerator Supplement (DAS)
 Total Funding - 120,000
 Portion of Funding Received - 120,000
 Funding Competitive?: Yes

2017/10 - 2021/9
 Co-investigator

Next Generation Catalytic Aftertreatment Technology for Exhaust Emission Control, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
 Strategic Partnership Grants (SPG)
 Total Funding - 427,330
 Portion of Funding Received - 100,000
 Funding Competitive?: Yes

Principal Applicant : Chin, Y. H.

2016/7 - 2021/6
 Principal Investigator

Computational Design and Discovery of Low Dimensional Materials for Solar Driven Hydrogen Production and CO₂ Conversion to Useful Chemical Fuels, Research Chair

Funding Sources:

Hart Foundation
 Erwin Edward Hart Endowed Professorship
 Total Funding - 225,000
 Portion of Funding Received - 225,000
 Funding Competitive?: No

2019/4 - 2020/3
 Principal Applicant

Integrated Computational Materials Engineering for Sustainable Energy & Lightweight Applications (Compute Canada Resource Allocation, in-kind funding), Grant

Funding Sources:

Compute Canada
 Resource Allocation
 Total Funding - 800,000
 Portion of Funding Received - 800,000
 Funding Competitive?: Yes

2017/7 - 2019/6 Co-investigator	<p>A Nanomanipulation-AFM System inside FIB-SEM for in-Situ Nanomaterial Characterization, Grant</p> <p>Funding Sources: Natural Sciences and Engineering Research Council of Canada (NSERC) Research Tools & Instruments (RTI) Total Funding - 311,073 Portion of Funding Received - 75,000 Funding Competitive?: Yes</p> <p>Principal Applicant : Liu, X.</p>
2016/7 - 2019/6 Principal Investigator	<p>Collaborative Learning Facility for Computational Materials Engineering, Grant</p> <p>Funding Sources: University of Toronto Dean's Strategic Fund Total Funding - 150,000 Portion of Funding Received - 150,000 Funding Competitive?: Yes</p>
2018/4 - 2019/4 Principal Applicant	<p>Integrated computational materials engineering for sustainable energy & lightweight applications (4039 core years computing allocation and 180 TB storage allocation), Grant</p> <p>Funding Sources: Compute Canada RAC Total Funding - 639,769 Portion of Funding Received - 639,769 Funding Competitive?: Yes</p>
2016/4 - 2019/3 Co-investigator	<p>A Versatile, Multifunctional System for Full Characterizations of Reaction Intermediates and Pathways for Sustainable Synthesis of Smart Materials and Value-added Chemicals, Grant</p> <p>Funding Sources: Natural Sciences and Engineering Research Council of Canada (NSERC) Research Tools & Instruments Total Funding - 126,428 Portion of Funding Received - 12,000 Funding Competitive?: Yes</p> <p>Principal Investigator : Chin, Y. H.</p>
2012/8 - 2018/10 Principal Investigator	<p>Mechanical Characterization Platform for Integrated Computational Materials Engineering Laboratory, Grant</p> <p>Funding Sources: Canada Foundation for Innovation (CFI) Infrastructure Operating Fund (IOF) Total Funding - 28,653 Portion of Funding Received - 28,653 Funding Competitive?: Yes</p> <p>Canada Foundation for Innovation (CFI) John R. Evans Leaders Fund Total Funding - 95,510 Portion of Funding Received - 95,510 Funding Competitive?: Yes</p> <p>Anton Paar GmbH Total Funding - 73,653</p>

Portion of Funding Received - 73,653
 Funding Competitive?: No
 Ontario Research Fund (ORF)
 Total Funding - 95,510
 Portion of Funding Received - 95,510
 Funding Competitive?: Yes

2015/7 - 2018/6
 Collaborator

High Performance PV Polysilicon and Ingot Pilot Plant, Contract

Funding Sources:

Sustainable Development Technology Canada
 Total Funding - 3,122,445
 Portion of Funding Received - 203,600
 Funding Competitive?: Yes

Co-investigator : Barati, M.; Chattopadhyay, K.; Hibbard, G. D.

2013/7 - 2018/6
 Co-investigator

Design and Manufacturing of Direct Micro and Long-fibre Lightweight Composites, Grant

Funding Sources:

Ford Motors Canada
 Total Funding - 2,418,000
 Portion of Funding Received - 50,000
 Funding Competitive?: Yes
 Natural Sciences and Engineering Research Council of Canada (NSERC)
 Automotive Partnership Canada
 Total Funding - 2,513,500
 Portion of Funding Received - 140,000
 Funding Competitive?: Yes

Principal Investigator : Sain, M.

2016/1 - 2018/6
 Principal Investigator

Generation and Characterization of High Performance PV Silicon, Grant

Funding Sources:

Ubiquity Solar Inc.
 Total Funding - 206,000
 Portion of Funding Received - 130,000
 Funding Competitive?: Yes
 Mathematics of Information Technology and Complex Systems (MITACS)
 Accelerate Cluster
 Total Funding - 453,333
 Portion of Funding Received - 240,000
 Funding Competitive?: Yes

Co-investigator : Glenn Hibbard; Kinnor Chattopadhyay; Mansoor Barati

2012/4 - 2018/3
 Principal Investigator

Enhancing the Performance Limits of Nanostructured Materials through Atomistic Modeling, Experimental Validation and Design Optimization, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
 Discovery (DGP)
 Total Funding - 144,000
 Portion of Funding Received - 120,000
 Funding Competitive?: Yes

2017/4 - 2018/3
 Principal Investigator

Integrated Computational Materials Engineering for Sustainable Energy & Lightweight Applications (4500 core years computing allocation and 300 TB storage allocation), Grant

Funding Sources:

Compute Canada
 RAC
 Total Funding - 818,622
 Portion of Funding Received - 818,622
 Funding Competitive?: Yes

2015/8 - 2017/12
 Co-investigator

The New CO2 Economy: Solar Energy Enabled Closed Carbon Cycle, Grant

Funding Sources:

Connaught Foundation (Ontario)
 Connaught Global Challenge Award
 Total Funding - 1,000,000
 Portion of Funding Received - 200,000
 Funding Competitive?: Yes

Principal Investigator : Ozin, G. A.

2013/7 - 2017/8
 Co-investigator

Bulk Metallic Glasses for Use in Gravity Gradiometer, Grant

Funding Sources:

Gedex Inc.
 Total Funding - 108,000
 Portion of Funding Received - 54,000
 Funding Competitive?: Yes
 Natural Sciences and Engineering Research Council of Canada (NSERC)
 CRD
 Total Funding - 323,900
 Portion of Funding Received - 161,950
 Funding Competitive?: Yes

Collaborator : Gedex Inc.;

Principal Investigator : Thorpe, S.J.

2016/1 - 2017/3
 Principal Investigator

Computational Discovery of Novel Catalytic Materials for Photo-excited CO2 Reduction, (In-kind grant for resource allocation), Grant

Funding Sources:

Compute Canada
 RAC
 Total Funding - 262,675
 Portion of Funding Received - 262,675
 Funding Competitive?: Yes

2016/5 - 2017/1
 Principal Investigator

Experimental Characterization and Modeling of Mechanical Properties of High and Intermediate Mn Steels, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
 Engage
 Total Funding - 25,000
 Portion of Funding Received - 25,000
 Funding Competitive?: Yes
 Collaborator : Hatch Ltd.

Under Review [n=3]

2024/4 - 2027/3
 Co-applicant

Functionally Graded Materials: A Novel Approach Based on Cold Spray Additive Manufacturing, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
Alliance
Total Funding - 492,000
Portion of Funding Received - 123,000
Funding Competitive?: Yes

Principal Applicant : Ali Dolatabadi

2023/4 - 2026/3
Co-applicant

Next Generation Additive Manufacturing: AI Driven Materials and Process Development, Grant

Funding Sources:

Ontario Research Fund (ORF)
Research excellence
Total Funding - 2,500,000
Portion of Funding Received - 200,000
Funding Competitive?: Yes

2019/4 - 2022/3
Co-investigator

In-situ Transmission Electron Microscope Nanoindenter and Tribometer, Grant

Funding Sources:

Natural Sciences and Engineering Research Council of Canada (NSERC)
RTI
Total Funding - 450,000
Portion of Funding Received - 150,000
Funding Competitive?: Yes

Student/Postdoctoral Supervision

Bachelor's [n=18]

2023/4 - 2024/8

Principal Supervisor

Pasha Ho (In Progress) , University of Toronto
Thesis/Project Title: Benchmarking ML models and databases for high entropy alloy catalysts
Present Position: UG Researcher in my lab

2019/9 - 2020/6

Principal Supervisor

Lyu, Tianyi (Completed) , University of Toronto
Thesis/Project Title: Machine learning driven discovery and design of high entropy alloys
Present Position: Doctoral student in another group, University of Toronto

2019/9 - 2020/6

Principal Supervisor

Xu, Anni (Completed) , University of Toronto
Thesis/Project Title: AI enabled design of catalysts for CO2 reduction
Present Position: Graduate student in my lab, University of Toronto

2019/9 - 2020/8

Principal Supervisor

Liu, Szu-Jia (Jessica) (Completed) , University of Toronto
Thesis/Project Title: Machine learning driven discovery and design of high entropy alloys
Present Position: Doctoral student in my lab, University of Toronto

2019/9 - 2020/6

Principal Supervisor

Chen, Gui (Completed) , University of Toronto
Thesis/Project Title: AI enabled design of catalysts for CO2 reduction
Present Position: Graduate student in my lab, University of Toronto

2019/5 - 2022/6

Principal Supervisor

Zhu, Julien (In Progress) , University of Toronto
Thesis/Project Title: Molecular dynamics simulations of irradiation effects in silicon carbide
Present Position: Undergraduate student, University of Toronto

2019/5 - 2022/6 Principal Supervisor	Cheng, Yu Hui (In Progress) , University of Toronto Thesis/Project Title: Computational design of 2D materials for CO2 reduction Present Position: Undergraduate student, University of Toronto
2019/5 - 2022/6 Principal Supervisor	Persaud, Daniel (In Progress) , University of Toronto Thesis/Project Title: Computational catalyst design Present Position: Undergraduate student, University of Toronto
2019/5 - 2022/6 Principal Supervisor	Sa, Jong Hyun (In Progress) , University of Toronto Thesis/Project Title: Computational catalyst design Present Position: Undergraduate student, University of Toronto
2019/4 - 2020/6 Principal Supervisor	Kaushik, Apurv (Completed) , University of Toronto Thesis/Project Title: Irradiation effects in 2D materials Present Position: Just completed
2018/9 - 2019/6 Principal Supervisor	Min, Rachel Wong (Completed) , University of Toronto Thesis/Project Title: Machine learning for structure-property relationships in metallic systems Present Position: Graduate student at École polytechnique fédérale de Lausanne
2017/9 - 2018/6 Principal Supervisor	Mohamed, Rahma (Completed) , University of Toronto Thesis/Project Title: Structure - mechanical property relationships for 2D materials Present Position: Undergraduate researcher in my lab
2017/9 - 2018/6 Principal Supervisor	Hirst, Nathan (Completed) , University of Toronto Thesis/Project Title: Finite element analysis of failure in biomedical hip implant Present Position: EIT at Arcon Forensic Engineers
2016/9 - 2017/9 Principal Supervisor	Pao, Wingyi (Roxana) (Completed) , University of Toronto Thesis/Project Title: Finite element analysis of damage behavior in composite helicopter blades Present Position: Graduate student, UOIT
2016/4 - 2019/6 Principal Supervisor	Banwait, Avinav (Completed) , University of Toronto Thesis/Project Title: Machine learning for structure-property relationships in metallic systems Present Position: Senior Systems Design Engineer at AMD
2016/4 - 2018/6 Principal Supervisor	Lu, Zhuole (Completed) , University of Toronto Thesis/Project Title: Computational design of catalytic materials to enable artificial photosynthesis Present Position: ML Developer at Wysom.AI
2014/5 - 2017/6 Principal Supervisor	Gao, Anthony (Completed) , University of Toronto Thesis/Project Title: Molecular dynamics simulations of Si nanowires coated with atomic layer deposition technique Present Position: Software Developer, ParseHub
2013/5 - 2017/5 Principal Supervisor	Alicandri, Robert (Completed) , University of Toronto Thesis/Project Title: Atomistic investigation of mechanical failure from curved grain boundaries in graphene Present Position: Engineer in industry

Master's Equivalent [n=1]

2017/2 - 2017/6 Principal Supervisor	Seebaluck, Antish, d'Arts Metiers Paris Tech. Thesis/Project Title: Molecular dynamics based nanoindentation analysis of Ni-Co nanolaminates, Visiting Masters student Present Position: Masters student, d'Arts Metiers Paris Tech.
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Master's non-Thesis [n=5]

2017/9 - 2018/11 Principal Supervisor	Hajiyev, Kamal (Completed) , University of Toronto Thesis/Project Title: Damage and failure analysis of composite structures Present Position: Masters student in my lab
2017/9 - 2018/6 Principal Supervisor	Ma, Xueqi (Completed) , University of Toronto Thesis/Project Title: Ab initio modeling of 2D materials for sunlight driven CO2 reduction Present Position: Associate, JTE Claims Consultants Ltd.
2017/9 - 2018/11 Principal Supervisor	Kumar, Vignesh (Completed) , University of Toronto Thesis/Project Title: Experimental evaluation of interfacial failure in nano Ni-Co coated additively manufactured hybrid structures Present Position: Just graduated
2017/1 - 2017/5 Principal Supervisor	Nicholson, Eric (Completed) , University of Toronto Thesis/Project Title: Ab initio molecular dynamics simulations of radiation damage in nuclear materials Present Position: MASc student in my lab
2016/9 - 2017/11 Principal Supervisor	Deng, Junwei (Completed) , University of Toronto Thesis/Project Title: Theoretical investigation of mechanical properties of one dimensional nanomaterials Present Position: Masters student in my lab, University of Toronto

Master's Thesis [n=12]

2021/9 - 2023/11 Principal Supervisor	Ethan Halpren (In Progress) , University of Toronto Thesis/Project Title: First-Principles and Machine Learning Investigation of Multi-Principal Element Materials for Hydrogen Generation and Storage Present Position: Graduate student in my lab
2021/5 - 2024/11 Principal Supervisor	Zachary Garipey (In Progress) , University of Toronto Thesis/Project Title: Design of Multi-component Alloy Catalysts Aided by Density Functional Theory and Machine Learning Present Position: Graduate student in my lab
2020/9 - 2023/8 Principal Supervisor	Rempel, Jacob (All But Degree) , University of Toronto Thesis/Project Title: Machine learning enabled development of all solid state electrolyte batteries Present Position: Ready to graduate
2019/9 - 2021/11 Principal Supervisor	Lu, Zhoule (Completed) , University of Toronto Thesis/Project Title: AI enabled screening and design of complex alloy catalysts Present Position: ML Developer at Wysom.AI
2017/9 - 2019/8 Principal Supervisor	Kavalsky, Lance (Completed) , University of Toronto Thesis/Project Title: Computational discovery and screening of novel 2D materials for metal-air batteries Present Position: PhD student at Carnegie Mellon University, USA
2017/9 - 2019/8 Principal Supervisor	Alicandri, Robert (Completed) , University of Toronto Thesis/Project Title: Multiscale modeling of metallurgical processing of solar grade silicon Present Position: Project engineer in nuclear industry
2017/6 - 2019/8 Principal Supervisor	Nicholson, Eric (Completed) , University of Toronto Thesis/Project Title: Atomistic modeling and experimental investigation of nuclear processes in fission and fusion materials Present Position: PhD student in my lab

2017/5 - 2019/8 Co-Supervisor	Huxter, William (Completed) , University of Toronto Thesis/Project Title: Electronic structure of nano-textured surfaces Present Position: PhD student at ETHZ, Switzerland
2016/9 - 2018/11 Principal Supervisor	Kumar, Ashok (Completed) , University of Toronto Thesis/Project Title: Multiscale modeling of failure in Ni-Co nanolaminates Present Position: Just graduated
2016/9 - 2018/11 Principal Supervisor	Agrawal, Pratyaksh (Completed) , University of Toronto Thesis/Project Title: Structure - mechanical property relationships for novel 2D transition metal dichalcogenides Present Position: Senior Investigator AML Risk, Scotiabank
2016/5 - 2018/6 Principal Supervisor	Grixti, Sean (Completed) , University of Toronto Thesis/Project Title: Ab-initio design of electrocatalysts for green energy Present Position: Strategic Business Development Manager, Li-Cycle Corp., Zurich, Switzerland
2014/9 - 2017/2 Principal Supervisor	Kumar, Mohit (Completed) , University of Toronto Thesis/Project Title: Multiscale modeling of mechanical and vibrational properties of bulk metallic glasses Present Position: Engineer, The Aquila Group

Doctorate [n=17]

2023/5 - 2028/4 Principal Supervisor	Mohammadhossein Ghoncheh (In Progress) , University of Toronto Thesis/Project Title: 2D high entropy materials for energy storage applications Present Position: Doctoral student in my lab
2022/5 - 2026/6 Principal Supervisor	Huang, Linke (In Progress) , University of Toronto Thesis/Project Title: Computational and experimental investigation of surface electronics of thin films Present Position: Doctoral student in my lab
2021/9 - 2026/8 Principal Supervisor	Demingos, Pedro Guerra (In Progress) , University of Toronto Thesis/Project Title: Surface Engineering non-van der Waals 2D Materials for Mechanical and Functional Applications Present Position: Doctoral student in my lab
2021/9 - 2026/8 Principal Supervisor	Xiang Ni (In Progress) , University of Toronto Thesis/Project Title: Designing Carbon Nanofibers-based Nanomaterials for Energy Applications Present Position: Doctoral student in my lab
2021/9 - 2027/8 Principal Supervisor	Adwitiya Rao (In Progress) , University of Toronto Thesis/Project Title: AI driven design and optimization of all solid state battery materials Present Position: Doctoral student in my lab
2020/9 - 2025/8 Principal Supervisor	Liu, Szu - Jia (Jessica) (In Progress) , University of Toronto Thesis/Project Title: Computational design of high entropy alloys for high temperature applications Present Position: Doctoral student in my lab, University of Toronto
2019/9 - 2024/8 Principal Supervisor	Nicholson, Eric (In Progress) , University of Toronto Thesis/Project Title: Atomistic level understanding of grain orientations on the irradiation hardening Present Position: PhD student in my lab, University of Toronto

2019/5 - 2022/9 Co-Supervisor	Chi, Lonxing (Completed) , University of Toronto Thesis/Project Title: 2D Surface Characterization and Analysis via STM and DFT Present Position: Research Scientist, OTI Lumionics, Toronto, Canada
2018/9 - 2024/6 Principal Supervisor	Hema Rajesh Nadella (In Progress) , University of Toronto Student Degree Expected Date: 2024/6 Thesis/Project Title: Machine learning based design and exploration of 2D materials Present Position: Doctoral researcher in my lab
2018/9 - 2024/6 Principal Supervisor	Abu Anand (In Progress) , University of Toronto Student Degree Expected Date: 2024/6 Thesis/Project Title: Ab-initio modeling of mechanical ductility in high entropy alloys Present Position: Doctoral researcher in my lab
2017/9 - 2022/2 Principal Supervisor	Najafi, Farzin (Completed) , University of Toronto Thesis/Project Title: Fatigue and fracture of graphene and graphene oxide nanomaterials Present Position: Advanced Packaging Engineer, GaN Systems Inc., Ottawa, Canada
2017/9 - 2024/6 Principal Supervisor	Choukir, Sahar (In Progress) , University of Toronto Student Degree Expected Date: 2024/6 Thesis/Project Title: Multiscale design and analysis of nano Ni-Co coated additively manufactured hybrid structures for aerospace applications Present Position: PhD student in my lab
2015/9 - 2023/6 Principal Supervisor	Dhaliwal, Gurjot (Completed) , University of Toronto Thesis/Project Title: Development of stochastic interatomic potential for molecular dynamics simulations of carbon and metallic nanomaterials Present Position: Co-founder and CTO, Phaseshift Technologies, Mississauga, Canada
2015/9 - 2021/6 Principal Supervisor	Yadav, Shwetank (Completed) , University of Toronto Thesis/Project Title: Multiscale modeling of manufacturing process for Silicon wafers Present Position: Applications Engineer at Micron Technologies, USA
2015/1 - 2020/6 Principal Supervisor	Sun, Hao (Completed) , University of Toronto Thesis/Project Title: Atomistic modeling of annealing detwinning in Ni based nanomaterials Present Position: Postdoctoral Fellow, Queens University
2014/10 - 2018/12 Principal Supervisor	Berton, Thomas (Completed) , University of Toronto Thesis/Project Title: Durability, structural integrity, and long-term performance of natural fiber polymer composites Present Position: Scientific Software Developer, Altim Group, Toulouse, France
2012/9 - 2017/4 Principal Supervisor	Daly, Matthew (Completed) , University of Toronto Thesis/Project Title: Multiscale modeling of mechanical failure in multilayered nanocrystalline alloy systems Present Position: Assistant Professor, Univ. of Illinois at Chicago, USA

Doctorate Equivalent [n=2]

2019/10 - 2021/8 Principal Supervisor	Chen, Dachang (Completed) , Wuhan University Thesis/Project Title: First principles investigations of novel materials for green energy applications Present Position: Doctoral student in my lab, University of Toronto
2019/7 - 2023/6 Principal Supervisor	Jiang, Ming (Completed) , University of Electronic Science and Technology of China Thesis/Project Title: Computational design of next generation materials for all solid state electrolyte batteries Present Position: Doctoral student in my lab, University of Toronto

Post-doctorate [n=6]

2021/3 - 2024/8 Principal Supervisor	Xue Yao (In Progress) , University of Toronto Thesis/Project Title: DFT simulations of high entropy materials for catalytic applications Present Position: PDF in my lab
2020/2 - 2024/5 Principal Supervisor	Chen, Li Xin (In Progress) , University of Toronto Thesis/Project Title: Experimental and computational development of high entropy alloy catalysts Present Position: PDF in my group
2019/10 - 2024/8 Principal Supervisor	Chen, Zhi Wen (In Progress) , University of Toronto Thesis/Project Title: Computational design of single atom and double atom catalysts for sustainable energy Present Position: Postdoctoral fellow in my lab
2016/11 - 2018/7 Principal Supervisor	Makaremi, Meysam (Completed) , University of Toronto Thesis/Project Title: Computational screening and design of nanomaterials for sunlight driven CO2 reduction Present Position: Process Modeling Development Engineer, Howmet Aerospace, USA
2016/10 - 2018/12 Principal Supervisor	Haldar, Sandip (Completed) , University of Toronto Thesis/Project Title: Multiscale experimentation and modeling of damage and failure in composite materials Present Position: Assistant Professor, Indian Institute of Technology Goa, India
2016/1 - 2021/6 Principal Supervisor	Mukherjee, Sankha (Completed) , University of Toronto Thesis/Project Title: Computational exploration and design of 2D materials for battery electrodes Present Position: Assistant Professor, Indian Institute of Technology - Kharagpur

Research Associate [n=1]

2016/11 - 2017/12 Principal Supervisor	Ghuman, Kulbir Kaur (Completed) , University of Toronto Thesis/Project Title: Ab initio design of photocatalysts for artificial photosynthesis Present Position: Assistant Professor at Institut national de la recherche scientifique (INRS), Montreal, Canada, International Institute for Carbon-Neutral Energy Research, Kyushu Univ., Japan
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International Collaboration Activities

2021/9 - 2025/7	Collaborator, China Prof. Qing Jiang, Jilin University. Collaborating on atomic catalysts.
2018/9 - 2024/8	Collaborator, United States of America Prof. Pulickel Ajayan, Rice University, Mechanics of two dimensional materials
2011/9 - 2024/6	Collaborator,, India Prof. PJ Guruprasad, Aerospace Engineering, Indian Institute of Technology - Bombay, Damage development in composite helicopter rotor blades
2016/3 - 2022/8	Collaborator,, India Prof. Dinesh Kumar Harursampath, Indian Institute of Science - Bangalore, Variational asymptotic method
2014/8 - 2019/6	Collaborator, United States of America Prof. Phanish Suryanarayana, Georgia Institute of Technology, Practical applications of large-scale density functional theory codes

Committee Memberships

2017/7	Co-chair, Research, Department of Materials Science & Engineering, University of Toronto Associate Chair
2016/9	Committee Member, Panelist for NSF Career Grant, National Science Foundation (NSF), USA
2015/12	Committee Member, Faculty Search Committee, Faculty of Applied Science & Engineering, University of Toronto
2012/4	Committee Member, Multidisciplinary Capstone Design Project Committee, Faculty of Applied Science & Engineering, University of Toronto
2014/6 - 2026/12	Committee Member, TMS - Integrated Computational Materials Engineering (ICME), The Minerals, Metals & Materials Society (TMS)
2015/9 - 2024/3	Committee Member, Compute Canada RAC Expert Review Committee, Compute Canada
2015/7 - 2017/6	Committee Member, First Year Undergraduate Curriculum Committee, Faculty of Applied Science & Engineering, University of Toronto
2015/7 - 2017/6	Committee Member, Teaching Methods & Resources Committee, Faculty of Applied Science & Engineering, University of Toronto

Other Memberships

2015/5 - 2024/6	Member, Professional Engineers Ontario
2012/6 - 2024/6	Professional Member, Materials Research Society
2007/7 - 2020/12	Lifetime Member, The Minerals, Metals & Materials Society (TMS)

Presentations

- (2019). Silicon nanoparticles-based photocatalysts for efficient CO₂ reduction. International Conference on Advances in Functional Materials in UCLA (AAAFM), Los Angeles, United States of America
Main Audience: Researcher
Invited?: Yes, Keynote?: No
- (2019). Potential of 2D Nanomaterials for sustainable energy storage. University of Toronto - Tokyo - McMaster (UT²-Mac) International Workshop, Toronto, Ontario, Canada
Main Audience: Knowledge User
Invited?: Yes, Keynote?: Yes
- (2019). Multiscale synergistic damage mechanics methodology for predicting progressive failure in composite structures. 148th TMS Annual Meeting, San Antonio, United States of America
Main Audience: Researcher
Invited?: Yes, Keynote?: No
- (2019). Computational design of 2D nanomaterials for sustainable energy. Canadian Society for Mechanical Engineering (CSME), London, Ontario, Canada
Main Audience: Knowledge User
Invited?: Yes, Keynote?: Yes

5. (2018). Computational discovery and design of nanomaterials for sustainable energy and lightweight transportation. Universidad Nacional Autónoma de México, Mexico City, Mexico
Main Audience: Knowledge User
Invited?: Yes, Keynote?: No
6. (2018). Size effects in mechanical properties of 2D materials. Computational Materials North Workshop, Montreal, Canada
Main Audience: Knowledge User
Invited?: Yes, Keynote?: Yes
7. (2018). Size effects in mechanical properties of graphene oxide nanosheets. Materials Science & Technology (MS&T) Conference, Columbus, United States of America
Main Audience: Researcher
Invited?: Yes, Keynote?: No
8. (2018). Materials modeling - What is the state of the art?: Challenges & Opportunities. Materials Assemblages Workshop, Toronto, Canada
Main Audience: Knowledge User
Invited?: Yes, Keynote?: No
9. (2017). Computational materials science: a new paradigm for discovery of next generation of materials technologies. Invited Talk, Galgotia Institute of Technology, Noida, India
Main Audience: Knowledge User
Invited?: Yes, Keynote?: No
10. (2017). Computational discovery and design of low-dimensional materials for lightweight transportation and sustainable energy. Invited Talk, Queens University, Kingston, Canada
Main Audience: Researcher
Invited?: Yes, Keynote?: No
11. (2017). Multiscale modeling of materials for sustainable transportation and energy applications. Invited Talk, Department of Mechanical Engineering, York University, Toronto, Canada
Main Audience: Knowledge User
Invited?: Yes, Keynote?: No
12. (2017). New insights into deformational mechanisms of materials and structures for sustainable transportation through multiscale modeling. Invited Talk, Indian Institute of Technology – Bombay, Mumbai, India
Main Audience: Researcher
Invited?: Yes, Keynote?: No
13. (2017). Computational design and discovery of emerging materials for sustainable energy, transportation and infrastructure. Invited Talk, Tata Research Development and Design Centre, Tata Consultancy Services, Pune, India
Main Audience: Researcher
Invited?: Yes, Keynote?: No

Broadcast Interviews

2015/04/02 - How to design materials of future using computers?, ICI Radio Canada, CBC
2015/04/02

Publications

Journal Articles

1. Yu, Ruizhi and Wang, Changhong and Duan, Hui and Jiang, Ming and Zhang, Anbang and Fraser, Adam and Zuo, Jiaxuan and Wu, Yanlong and Sun, Yipeng and Zhao, Yang and others. (2023). Manipulating Charge-Transfer Kinetics of Lithium-Rich Layered Oxide Cathodes in Halide All-Solid-State Batteries. *Advanced Materials*. 35(5): 2370029.
Published
Refereed?: Yes
2. Choukir, Sahar and van Egmond, Derek Aranguren and Hatton, Benjamin D and Hibbard, Glenn D and Singh, Chandra Veer. (2023). The interplay between constituent material and architectural disorder in bioinspired honeycomb structures. *International Journal of Engineering Science*. 188: 103863.
Published
Refereed?: Yes
3. Huo, Hanyu and Jiang, Ming and Mogwitz, Boris and Sann, Joachim and Yusim, Yuriy and Zuo, Tong-Tong and Moryson, Yannik and Minnmann, Philip and Richter, Felix H and Singh, Chandra Veer and others. (2023). Interface Design Enabling Stable Polymer/Thiophosphate Electrolyte Separators for Dendrite-Free Lithium Metal Batteries. *Angewandte Chemie International Edition*.
Published
Refereed?: Yes
4. Kumral, B and Demingos, PG and Cui, T and Serles, P and Barri, N and Singh, CV and Filleter, T. (2023). Defect engineering of graphene for dynamic reliability. *Small*. : 2302145.
Published
Refereed?: Yes
5. Yao, Xue and Zhang, Zhiming and Chen, LiXin and Chen, Zhi-Wen and Zhu, Yong-Fu and Singh, Chandra Veer. (2023). Work Function-Tailored Nitrogenase-like Fe Double-Atom Catalysts on Transition Metal Dichalcogenides for Nitrogen Fixation. *ACS Sustainable Chemistry & Engineering*. 11(13): 4990-4997.
Published
Refereed?: Yes
6. Xue, Hongyao and Meng, Alan and Lian, Tongtong and Yang, Tongqing and Gao, Jiangshan and Singh, Chandra Veer and Geng, Zhihong and Chen, Lixin and Li, Zhenjiang. (2023). Co--Pyridinic-N Bond Constructed at the Interface of Co x P and N-Doped Carbon to Effectively Facilitate Oxygen Reduction. *ACS Sustainable Chemistry & Engineering*. 11(13): 5238-5249.
Published
Refereed?: Yes
7. Garipey, Zachary and Chen, Guiyi and Xu, Anni and Lu, Zhuole and Chen, Zhi Wen and Singh, Chandra Veer. (2023). Machine learning assisted binary alloy catalyst design for the electroreduction of CO₂ to C₂ products. *Energy Advances*. 2(3): 410--419.
Published
Refereed?: Yes
8. Yang, Xiaofei and Gao, Xuejie and Jiang, Ming and Luo, Jing and Yan, Jitong and Fu, Jiamin and Duan, Hui and Zhao, Shangqian and Tang, Yongfu and Yang, Rong and others. (2023). Grain Boundary Electronic Insulation for High-Performance All-Solid-State Lithium Batteries. *Angewandte Chemie*. 135(5): e202215680.
Published
Refereed?: Yes

9. Gao, Chan and Singh, Chandra Veer. (2023). Mechanical properties and magnetic and electronic properties tuned via strain in two-dimensional non-van der Waals hematene. *Nuclear Analysis*. 2(1): 100061.
Published
Refereed?: Yes
10. Wang, D and Chen, ZW and Wu, Y and Huang, YC and Tao, L and Chen, J and Dong, CL and Singh, CV and Wang, S. (2023). Structurally ordered high-entropy intermetallic nanoparticles with enhanced C--C bond cleavage for ethanol oxidation. *SmartMat*. 4(1): e1117.
Published
Refereed?: Yes
11. Jiang, Ming and Guo, Xing-Can and Zu, Xiao-Tao and Singh, Chandra Veer. (2023). The effects of point defects on thermal-mechanical properties of BiCuOTe: a first-principles study. *Physical Chemistry Chemical Physics*. 25(15): 10715--10725.
Published
Refereed?: Yes
12. Nabil, Shariful Kibria and Roy, Soumyabrata and Algozeeb, Wala Ali and Al-Attas, Tareq and Bari, Md Abdullah Al and Zeraati, Ali Shayesteh and Kannimuthu, Karthick and Demingos, Pedro Guerra and Rao, Adwitiya and Tran, Thien N and others. (2023). Bifunctional Gas Diffusion Electrode Enables In-situ Separation and Conversion of CO₂ to Ethylene from Dilute Stream. *Advanced Materials*. : 2300389.
Published
Refereed?: Yes
13. Gao, Xuejie and Yang, Xiaofei and Jiang, Ming and Zheng, Matthew and Zhao, Yang and Li, Ruying and Ren, Wenfeng and Huang, Huan and Sun, Runcang and Wang, Jiantao and others. (2023). Fast Ion Transport in Li-Rich Alloy Anode for High-Energy-Density All Solid-State Lithium Metal Batteries. *Advanced Functional Materials*. 33(7): 2209715.
Published
Refereed?: Yes
14. Dhaliwal, Gurjot and Anand, Abu and Nair, Prasanth B and Singh, Chandra Veer. (2023). Sparse random Fourier features based interatomic potentials for high entropy alloys. *arXiv preprint arXiv:2302.06844*.
Submitted
Refereed?: Yes
15. Wang, Dongdong and Chen, Zhi-Wen and Gu, Kaizhi and Chen, Chen and Liu, Yingying and Wei, Xiaoxiao and Singh, Chandra Veer and Wang, Shuangyin. (2023). Hexagonal Cobalt Nanosheets for High-Performance Electrocatalytic NO Reduction to NH₃. *Journal of the American Chemical Society*. 145(12): 6899--6904.
Published
Refereed?: Yes
16. Varshney, S and Chi, L and Singh, CV and Nogami, J. (2022). Atomic structure of PbBr₂ thin films on Ag (111). *Solid State Communications*. 343: 114651.
Published
Refereed?: Yes
17. del Carpio-Perochena, A and Nicholson, E and Singh, CV and Camilleri, J and Kishen, A. (2022). Impact of dentin conditioning and sealer modification with chitosan-hydroxyapatite nanocomplexes on the antibacterial and mechanical characteristics of root dentin. *Journal of Endodontics*. 48(10): 1319--1326.
Published
Refereed?: Yes

18. Lu, Z and Adeli, P and Yim, CH and Jiang, M and Rempel, J and Chen, ZW and Yadav, S and Mercier, P and Abu-Lebdeh, Y and Singh, CV. (2022). Automatically Capturing Key Features for Predicting Superionic Conductivity of Solid-State Electrolytes Using a Neural Network. *ACS Applied Energy Materials*. 5(7): 8042--8048.
Published
Refereed?: Yes
19. Dumont, A and Nicholson, E and Qiu, C and Pan, J and Gariepy, Z and Du, S and Howe, J and Singh, CV and Lu, ZH. (2022). Restructuring and Reshaping of CsPbX₃ Perovskites by Lithium Salts. *Advanced Materials Interfaces*. 9(30): 2201296.
Published
Refereed?: Yes
20. Jiang, M and Chen, ZW and Rao, A and Chen, LX and Zu, XT and Singh, CV. (2022). Se-doped Li₆PS₅Cl and Li_{5.5}PS_{4.5}Cl_{1.5} with improved ionic conductivity and interfacial compatibility: a high-throughput DFT study. *Journal of Materials Chemistry C*. 10(48): 18294--18302.
Published
Refereed?: Yes
21. Taheri, A and Pisana, S and Singh, CV. (2022). Extraordinary lattice thermal conductivity of gold sulfide monolayers. *Nanoscale Advances*. 4(13): 2873--2883.
Published
Refereed?: Yes
22. Serles, P and Hamidinejad, M and Demingos, PG and Ma, L and Barri, N and Taylor, H and Singh, CV and Park, CB and Filleter, T. (2022). Friction of Ti₃C₂T_x MXenes. *Nano letters*. 22(8): 3356--3363.
Published
Refereed?: Yes
23. Islam, MA and Serles, P and Kumral, B and Demingos, P G and Qureshi, T and Meiyazhagan, AK and Puthirath, AB and Abdullah, MSB and Faysal, SR and Ajayan, PM and others. (2022). Exfoliation mechanisms of 2D materials and their applications. *Applied Physics Reviews*. 9(4)
Published
Refereed?: Yes
24. Chen, LX and Chen, ZW and Yao, X and Su, B and Chen, W and Pang, X and Kim, KS and Singh, CV. (2022). High-entropy alloy catalysts: high-throughput and machine learning-driven design. *J. Mater. Inform.* 2(4): 19.
Published
Refereed?: Yes
25. Chen, ZW and Gariepy, Z and Chen, LX and Yao, X and Anand, A and Liu, SJ and Tetsassi Feugmo, CG and Tamblyn, I and Singh, CV. (2022). Machine-Learning-Driven High-Entropy Alloy Catalyst Discovery to Circumvent the Scaling Relation for CO₂ Reduction Reaction. *ACS Catalysis*. 12(24): 14864--14871.
Published
Refereed?: Yes
26. Cui, T and Mukherjee, S and Onodera, M and Wang, G and Kumral, B and Islam, A and Shayegannia, M and Krishnan, G and Barri, N and Serles, P and others. (2022). Mechanical reliability of monolayer MoS₂ and WSe₂. *Matter*. 5(9): 2975--2989.
Published
Refereed?: Yes
27. Chi, L and Nogami, J and Singh, CV. (2022). Phase Transformation-Induced Quantum Dot States on the Bi/Si (111) Surface. *ACS Applied Materials & Interfaces*. 14(31): 36217--36226.
Published
Refereed?: Yes

28. Gao, C and Yang, X and Jiang, M and Chen, LX and Chen, ZW and Singh, CV. (2022). Machine learning-enabled band gap prediction of monolayer transition metal chalcogenide alloys. *Physical Chemistry Chemical Physics*. 24(7): 4653--4665.
Published
Refereed?: Yes
29. Verma, D and Kumar, P and Mukherjee, S and Thakur, D and Singh, CV and Balakrishnan, V. (2022). Interplay between Thermal Stress and Interface Binding on Fracture of WS₂ Monolayer with Triangular Voids. *ACS Applied Materials & Interfaces*. 14(14): 16876--16884.
Published
Refereed?: Yes
30. Serles, P and Nicholson, E and Tam, J and Barri, N and Chemin, JB and Wang, G and Michel, Y and Singh, CV and Choquet, P and Saulot, A and others. (2022). High Performance Space Lubrication of MoS₂ with Tantalum. *Advanced Functional Materials*. 32(20): 2270117.
Published
Refereed?: Yes
31. Miller, KA and Alemany, LB and Roy, S and Yan, Q and Demingos, PG and Singh, CV and Alahakoon, S and Egap, E and Thomas, EL and Ajayan, PM. (2022). High-Strength, Microporous, Two-Dimensional Polymer Thin Films with Rigid Benzoxazole Linkage. *ACS Applied Materials & Interfaces*. 14(1): 1861--1873.
Published
Refereed?: Yes
32. Dhaliwal, G and Nair, PB and Singh, CV. (2022). Machine learned interatomic potentials using random features. *npj Computational Materials*. 8(1): 7.
Published
Refereed?: Yes
33. Qureshi, T and Wang, G and Mukherjee, S and Islam, MA and Filleter, T and Singh, CV and Panesar, DK. (2022). Graphene-based anti-corrosive coating on steel for reinforced concrete infrastructure applications: Challenges and potential. *Construction and Building Materials*. 351: 128947.
Published
Refereed?: Yes
34. Deng, S and Jiang, M and Chen, N and Li, W and Zheng, Ma and Chen, W and Li, R and Huang, H and Wang, J and Singh, CV and others. (2022). Regulating Electronic Conductivity at Cathode Interface for Low-Temperature Halide-Based All-Solid-State Batteries. *Advanced Functional Materials*. 32(45): 2205594.
Published
Refereed?: Yes
35. Prakash, A and Tak, TN and Anand, A and Pai, NN and Narayana Murty, SVS and Singh, CV and Guruprasad, PJ and Samajdar, I. (2022). Mechanistic origin of orientation-dependent substructure evolution in aluminum and aluminum-magnesium alloys. *Metallurgical and Materials Transactions A*. 53(7): 2689--2707.
Published
Refereed?: Yes
36. Ma, H and Chen, ZW and Wang, Z and Singh, CV and Jiang, Q. (2022). Interface engineering of Co/CoMoN/NF heterostructures for high-performance electrochemical overall water splitting. *Advanced Science*. 9(11): 2105313.
Published
Refereed?: Yes

37. Akhshik, M and Bilton, A and Tjong, J and Singh, CV and Faruk, O and Sain, M. (2022). Prediction of greenhouse gas emissions reductions via machine learning algorithms: Toward an artificial intelligence-based life cycle assessment for automotive lightweighting. *Sustainable Materials and Technologies*. 31: e00370.
Published
Refereed?: Yes
38. Chen, D and Mukherjee, S and Zhang, C and Li, Y and Xiao, B and Singh, CV. (2022). Two-dimensional square metal organic framework as promising cathode material for lithium-sulfur battery with high theoretical energy density. *Journal of Colloid and Interface Science*. 613: 435--446.
Published
Refereed?: Yes
39. Pakharenko, V and Dias, OAT and Mukherjee, S and Konar, S and Singh, CV and Oksman, K and Sain, M. (2022). Chemical and molecular structure transformations in atomistic conformation of cellulose nanofibers under thermal environment. *npj Materials Degradation*. 6(1): 16.
Published
Refereed?: Yes
40. Deng, S and Jiang, M and Rao, A and Lin, X and Doyle-Davis, K and Liang, J and Yu, C and Li, R and Zhao, S and Zhang, L and others. (2022). Fast-Charging Halide-Based All-Solid-State Batteries by Manipulation of Current Collector Interface. *Advanced Functional Materials*. 32(25): 2200767.
Published
Refereed?: Yes
41. Wang, G and Najafi, F and Ho, K and Hamidinejad, M and Cui, T and Walker, GC and Singh, CV and Filleter, T. (2022). Mechanical size effect of freestanding nanoconfined polymer films. *Macromolecules*. 55(4): 1248--1259.
Published
Refereed?: Yes
42. Han, Gao-Feng and Li, Feng and Chen, Zhi-Wen and Coppex, Claude and Kim, Seok-Jin and Noh, Hyuk-Jun and Fu, Zhengping and Lu, Yalin and Singh, Chandra Veer and Siahrostami, Samira and others. (2021). *Mechanochemistry for ammonia synthesis under mild conditions*. *Nature Nanotechnology*. 16(3): 325-330.
Published
Refereed?: Yes
43. Gao, C and Yang, X and Jiang, M and Chen, LX and Chen, ZW and Singh, CV. (2021). Synergistic vacancy defects and mechanical strain for the modulation of the mechanical, electronic and optical properties of monolayer tungsten disulfide. *Physical Chemistry Chemical Physics*. 23(10): 6298--6308.
Published
Refereed?: Yes
44. Wang, Dongdong and Chen, Zhiwen and Huang, Yu-Cheng and Li, Wei and Wang, Juan and Lu, Zhuole and Gu, Kaizhi and Wang, Tehua and Wu, Yujie and Chen, Chen and others. (2021). *Tailoring lattice strain in ultra-fine high-entropy alloys for active and stable methanol oxidation*. *Science China Materials*. : 1-13.
Published
Refereed?: Yes
45. Nicholson, Eric and Serles, Peter and Wang, Guorui and Filleter, Tobin and Davis, James W and Singh, Chandra Veer. (2021). *Low energy proton irradiation tolerance of molybdenum disulfide lubricants*. *Applied Surface Science*. 567: 150677.
Published
Refereed?: Yes

46. Liang, J and Chen, D and Adair, K and Sun, Q and Holmes, N G and Zhao, Y and Sun, Y and Luo, J and Li, R and Zhang, Li and others. (2021). Insight into prolonged cycling life of 4 V all-solid-state polymer batteries by a high-voltage stable binder. *Advanced Energy Materials*. 11(1): 2002455.
Published
Refereed?: Yes
47. Taheri, Armin and Pisana, Simone and Singh, Chandra Veer. (2021). *Importance of quadratic dispersion in acoustic flexural phonons for thermal transport of two-dimensional materials*. *Physical Review B*. 103(23): 235426.
Published
Refereed?: Yes
48. Chi, Longxing and Singh, Chandra Veer and Nogami, Jun. (2021). *Quantum well states and sizable Rashba splitting on Pb induced α -phase Bi/Si (111) surface reconstruction*. *Nanoscale*.
Published
Refereed?: Yes
49. Serles, P and Arif, T and Puthirath, AB and Yadav, S and Wang, G and Cui, T and Balan, A P and Yadav, TP and Thibeorchews, P and Chakingal, N and others. (2021). Friction of magnetene, a non--van der Waals 2D material. *Science advances*. 7(47): eabk2041.
Published
Refereed?: Yes
50. Chen, Li Xin and Jiang, Ming and Lu, Zhuole and Gao, Chan and Chen, Zhi Wen and Singh, Chandra Veer. (2021). *Two-dimensional graphdiyne-confined platinum catalyst for hydrogen evolution and oxygen reduction reactions*. *ACS Applied Materials & Interfaces*.
Published
Refereed?: Yes
51. Gao, Chan and Yang, Xiaoyong and Jiang, Ming and Chen, Lixin and Chen, Zhiwen and Singh, Chandra Veer. (2021). *Defect evolution behaviors from single sulfur point vacancies to line vacancies in monolayer molybdenum disulfide*. *Physical Chemistry Chemical Physics*. 23(35): 19525-19536.
Published
Refereed?: Yes
52. Chen, Zhi Wen and Lu, Zhuole and Chen, Li Xin and Jiang, Ming and Chen, Dachang and Singh, Chandra Veer. (2021). *Machine-learning-accelerated discovery of single-atom catalysts based on bidirectional activation mechanism*. *Chem Catalysis*. 1(1): 183-195.
Published
Refereed?: Yes
53. Sun, Hao and Singh, Chandra Veer. (2021). *A molecular dynamics study of dislocation ejection and shear coupling associated with incoherent twin boundary migration*. *Materialia*. 16: 101111.
Published
Refereed?: Yes
54. Ng, Kok Long and Lu, Zhuole and Wang, Yijia and Singh, Chandra Veer and Azimi, Gisele. (2021). Fundamental insights into electrical and transport properties of chloroaluminate ionic liquids for aluminum-ion batteries. *The Journal of Physical Chemistry C*. 125(28): 15145-15154.
Published
Refereed?: Yes
55. Chi, Longxing and Nogami, Jun and Singh, Chandra Veer. (2021). Bias dependence and defect analysis of Bi on Si (111) 3x3 β -phase. *Physical Review B*. 103(7): 075405.
Published
Refereed?: Yes

56. Yadav, Shwetank and Arif, Taib and Wang, Guorui and Sodhi, Rana NS and Cheng, Yu Hui and Filleter, Tobin and Singh, Chandra Veer. (2021). Interfacial interactions and tribological behavior of metal-oxide/2D-material contacts. *Tribology Letters*. 69(3): 1-11.
Published
Refereed?: Yes
57. van Egmond, D A and Yu, B and Choukir, S and Fu, S and Singh, CV and Hibbard, G and Hatton, BD and others. (2021). The benefits of structural disorder in natural cellular solids. *arXiv preprint arXiv:2110.04607*.
Submitted
Refereed?: Yes
58. Akhshik, M and Panthapulakkal, S and Tjong, J and Bilton, A and Singh, CV and Sain, M. (2021). Cross-country analysis of life cycle assessment--based greenhouse gas emissions for automotive parts: Evaluation of coefficient of country. *Renewable and Sustainable Energy Reviews*. 138: 110546.
Published
Refereed?: Yes
59. Pakharenko, Viktoriya and Mukherjee, Sankha and Dias, Otavio Augusto Tilton and Wu, Crystal and Manion, Joseph and Singh, Chandra Veer and Seferos, Dwight and Tjong, Jimi and Oksman, Kristiina and Sain, Mohini. (2021). Thermoconformational behavior of cellulose nanofiber films as a device substrate and their superior flexibility and durability to glass. *ACS Applied Materials & Interfaces*. 13(34): 40853--40862.
Published
Refereed?: Yes
60. Chen, LX and Wen, Z and Chen, ZW and Singh, CV and Jiang, Q. (2021). Insights into oxygen activation on metal clusters for catalyst design. *Journal of Materials Chemistry A*. 9(19): 11726--11733.
Published
Refereed?: Yes
61. Li, Jian and Chen, Li Xin and Liu, Xiao Xuan and Wen, Zi and Singh, Chandra Veer and Yang, Chun Cheng and Jiang, Qing. (2021). Eggshell-like MoS₂ nanostructures with negative curvature and stepped faces for efficient hydrogen evolution reactions. *ACS Applied Nano Materials*. 4(12): 14086--14093.
Published
Refereed?: Yes
62. Feugmo, Conrard Giresse Tetsassi and Ryczko, Kevin and Anand, Abu and Singh, Chandra Veer and Tamblyn, Isaac. (2021). *Neural evolution structure generation: High Entropy Alloys*. *Journal of Chemical Physics*. 155: 044102.
Published
Refereed?: Yes
63. Guo, C and Liu, S and Chen, ZW and Li, B and Chen, LX and Singh, CV and Liu, B and Mao, Q. (2021). How does mass transfer influence electrochemical carbon dioxide reduction reaction? A case study of Ni molecular catalyst supported on carbon. *Chemical Communications*. 57(11): 1384--1387.
Published
Refereed?: Yes
64. Taheri, Armin and Singh, Chandra Veer. (2021). *Anisotropic phonon thermal transport in nitrophosphorene monolayer*. *Physical Review Materials*. 5(3): 034009.
Published
Refereed?: Yes
65. Najafi, Farzin and Wang, Guorui and Cui, Teng and Anand, Abu and Mukherjee, Sankha and Filleter, Tobin and Sain, Mohini and Singh, Chandra Veer. (2021). *Fatigue resistance of atomically thin graphene oxide*. *Carbon*. 183: 780-788.
Published
Refereed?: Yes

66. Sun, Hao and Agrawal, Pratyaksh and Singh, Chandra Veer. (2021). *A first-principles study of the relationship between modulus and ideal strength of single-layer, transition metal dichalcogenides*. Materials Advances.
Published
Refereed?: Yes
67. Wang, Changhong and Hwang, Sooyeon and Jiang, Ming and Liang, Jianwen and Sun, Yipeng and Adair, Keegan and Zheng, Matthew and Mukherjee, Sankha and Li, Xiaona and Li, Ruying and others. (2021). *Deciphering interfacial chemical and electrochemical reactions of sulfide-based all-solid-state batteries*. Advanced Energy Materials. : 2100210.
Published
Refereed?: Yes
68. Wang, C., Liang, J., Jiang, M., Li, X., Mukherjee, S., Adair, K., Zheng, M., Zhao, Y., Zhao, F., Zhang, S., Li, R., Huang, H., Zhao, S., Zhang, S., Lu, S., Singh, C. V., Sun, X. (2020). *Interface-assisted in-situ growth of halide electrolytes eliminating interfacial challenges of all-inorganic solid-state batteries*. Nano Energy. 76: 105015.
Published
Refereed?: Yes
69. Yang, X., Gao, X., Mukherjee, S., Doyle-Davis, K., Fu, J., Li, W., Sun, Q., Zhao, F., Jiang, M., Hu, Y., Huang, H., Li, Zhang, L., Lu, S., Li, R., Sham, T.K., Singh, C. V., Sun, X. (2020). *Phase evolution of a prenucleator for fast Li nucleation in all-solid-state lithium batteries*. Advanced Energy Materials. 10(37): 2001191.
Published
Refereed?: Yes
70. Najafi, F., Wang, G., Mukherjee, S., Cui, T., Filleter, T., Singh, C. V. (2020). *Toughening of graphene-based polymer nanocomposites via tuning chemical functionalization*. Composites Science and Technology. 194: 108140.
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