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EDUCATION

Ph.D. in Mechanical Engineering from **McGill University**, Canada

M. Tech in Materials Science from **Indian Institute of Technology Bombay**, India

B.E. in Metallurgical and Materials Engineering from **Bengal Engineering and Science University** (Currently IIEST), Shibpur, India

PROFESSIONAL EXPERIENCE

Assistant Professor (December 2020 - present): **Indian Institute of Technology Kharagpur**, Department of Metallurgical and Materials Engineering

Postdoctoral fellow (February 2016- September 2020): **University of Toronto**, Canada

Assistant manager (July 2007-July2008): **Bharat Aluminium Company Ltd.** (BALCO), India

RESEARCH PROFILE (MATERIALS SCIENCE)

Areas of specialization:

I. *Computational modelling (density functional theory, molecular dynamics)*
II. *Light materials for structural applications (2D Materials)*
III. *Energy storage (rechargeable batteries, hydrogen fuel)*
IV. *Damping (internal friction) in nanodevices*

Current areas of research:

A. *Mechanics of graphene and its derivatives*
B. *Computational screening of electrode materials for alkali-ion, Li-S, and Li-air batteries*
C. *Design and discovery of solid-state electrolytes*
D. *Materials for hydrogen storage*
E. *Energy dissipation in nanoresonators*

RESEARCH THEMES

Mechanical properties of 2D materials: Since the synthesis of graphene, two-dimensional (2D) materials have revolutionized the field of materials science. While graphene is one of the strongest materials known to mankind with a strength of 100 GPa, it suffers from a poor fracture toughness (G_{IC}~ 16 J/m^2). Moreover, other than graphene, carbon has more than 30 polymorphs for which there exists no structure-property relationships. Finally, in real-life applications graphene-based systems are often subjected to a large cyclic stress. However, we do not know yet if these atomically thin materials are immune from fatigue failure? If not, what is the fatigue life and underlying damage mechanisms?

Materials for advanced rechargeable energy storage: A core challenge to scientists and engineers in the 21st Century is the development of energy-efficient systems and structures to mitigate global warming. Rechargeable batteries can store energy from renewable sources and discharge for hundreds of cycles. To improve the electrochemical performance of batteries (e.g., improve capacity and kinetics of alkali-

ion batteries and reduce shuttle effect in Li-S batteries), we require to find efficient electrode materials. With the ever-growing number of candidate materials, particularly 2D materials, search, develop and characterization of potential candidates can be challenging, time consuming and costly. In this context, atomistic simulations can be game changing for screening futuristic electrode materials.

Internal friction in nanoresonators: Silicon-based nanoresonators are common, operate at very high frequencies (in the GHz regime) and are ultrasensitive. The performance of these devices can be further improved by reducing materials damping and internal friction. Difficulties in studying internal friction in nanoresonators using experiments arise from their small size and the simultaneous existence of several mechanisms. As a result, despite of a lot of research activity a detailed microscopic understanding of the mechanisms of material damping is still illusive. In this pursuit, MD simulations can be particularly empowering, but it is not clear what are the methods for simulating damping using MD? *Furthermore, what are the mechanisms of material damping in single-crystal silicon, amorphous silicon, and amorphous silica nanoresonators?*

AWARDS and ACHIEVEMENTS

- *J. W. McConnell Memorial Fellowship:* McGill University (2012-13)
- *Rio Tinto - Richard Evans Graduate Fellowship:* McGill University (2011-12)
- *Engineering Recruitment Fund:* McGill University (2010-11)
- Obtained scholarship from Ministry of Human Resource Development, India, for graduate studies at IIT Bombay (August 2008 - June 2010)
- Ranked *first* in the M. Tech. program (IIT Bombay) with a CGPA of 9.59

PUBLICATIONS

2020

[J1] Yang, X.; Jiang, M.; Gao, X.; Bao, D.; Sun, Q.; Holmes, N.; Duan, H.; Mukherjee, S.; Adair, K.; Zhao, C., Determining the limiting factor of the electrochemical stability window for PEO-based solid polymer electrolytes: main chain or terminal–OH group? *Energy & Environmental Science* **2020,** *13* (5), 1318-1325.

[J2] Yang, X.; Gao, X.; Mukherjee, S.; Doyle-Davis, K.; Fu, J.; Li, W.; Sun, Q.; Zhao, F.; Jiang, M.; Hu, Y., Phase Evolution of a Prenucleator for Fast Li Nucleation in All-Solid-State Lithium Batteries. *Advanced Energy Materials* **2020,** *10* (37), 2001191.

[J3] Wang, C.; Liang, J.; Jiang, M.; Li, X.; Mukherjee, S.; Adair, K.; Zheng, M.; Zhao, Y.; Zhao, F.; Zhang, S., Interface-assisted in-situ growth of halide electrolytes eliminating interfacial challenges of all-inorganic solid-state batteries. *Nano Energy* **2020,** *76*, 105015.

[J4] 4. Qian, C.; Zhao, J.; Sun, Y.; Lee, H. R.; Luo, L.; Makaremi, M.; Mukherjee, S.; Wang, J.; Zu, C.; Xia, M., Electrolyte-Phobic Surface for the Next-Generation Nanostructured Battery Electrodes. *Nano Letters* **2020,** *20* (10), 7455-7462.

[J5] Phull, J.; Egas, J.; Barui, S.; Mukherjee, S.; Chattopadhyay, K., An Application of Decision Tree-Based Twin Support Vector Machines to Classify Dephosphorization in BOF Steelmaking. *Metals* **2020,** *10* (1), 25.

[J6] Najafi, F.; Wang, G.; Mukherjee, S.; Cui, T.; Filleter, T.; Singh, C. V., Toughening of graphene-based polymer nanocomposites via tuning chemical functionalization. *Composites Science and Technology* **2020,** *194*, 108140.

[J7] Mukherjee, S.; Kavalsky, L.; Chattopadhyay, K.; Singh, C. V., Dramatic improvement in the performance of graphene as Li/Na battery anodes with suitable electrolytic solvents. *Carbon* **2020,** *161*, 570-576.

[J8] Mukherjee, S.; Alicandri, R.; Singh, C. V., Strength of graphene with curvilinear grain boundaries. *Carbon* **2020,** *158*, 808-817.

[J9] Kavalsky, L.; Mukherjee, S.; Singh, C. V., Compression-induced resistance of singlet oxygen dissociation on phosphorene. *Physical Review Materials* **2020,** *4* (2), 021001.

Selected for Editor's Suggestions by Physical Review Materials

[J10] Jiang, M.; Mukherjee, S.; Chen, Z. W.; Chen, L. X.; Li, M. L.; Xiao, H. Y.; Gao, C.; Singh, C. V., Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. *Physical Chemistry Chemical Physics* **2020,** *22* (39), 22758-22767.

[J11] Cui, T.; Mukherjee, S.; Sudeep, P. M.; Colas, G.; Najafi, F.; Tam, J.; Ajayan, P. M.; Singh, C. V.; Sun, Y.; Filleter, T., Fatigue of graphene. **Nature materials** **2020,** *19* (4), 405-411.

Highlighted by ***Phys.org***. Web Link,
https://phys.org/news/2020-01-stress-reveals-graphene-wont-pressure.html
Highlighted by ***Nanowerk.*** Web Link,
https://www.nanowerk.com/nanotechnology-news2/newsid=54452.php

2019

[J12] Sun, H.; Mukherjee, S.; Shi, Z.; Singh, C. V., Elastomer-like deformation in high-Poisson's-ratio graphene allotropes may allow tensile strengths beyond theoretical cohesive strength limits. *Carbon* **2019,** *143*, 752-761.

[J13] Barui, S.; Mukherjee, S.; Srivastava, A.; Chattopadhyay, K., Understanding dephosphorization in basic oxygen furnaces (BOFs) using data driven modeling techniques. *Metals* **2019,** *9* (9), 955.

2018

[J14] Trudeau, C.; Dion-Bertrand, L.-I.; Mukherjee, S.; Martel, R.; Cloutier, S. G., Electrostatic deposition of large-surface graphene. *Materials* **2018,** *11* (1), 116.

[J15] Mukherjee, S.; Kavalsky, L.; Singh, C. V., Ultrahigh storage and fast diffusion of Na and K in blue phosphorene anodes. *ACS applied materials & interfaces* **2018,** *10* (10), 8630-8639.

[J16] Mukherjee, S.; Kavalsky, L.; Chattopadhyay, K.; Singh, C. V., Adsorption and diffusion of lithium polysulfides over blue phosphorene for Li–S batteries. *Nanoscale* **2018,** *10* (45), 21335-21352.

Selected for *Editor's Choice*: 2D Materials for Energy Storage and Conversion

[J17] Mukherjee, S.; Banwait, A.; Grixti, S.; Koratkar, N.; Singh, C. V., Adsorption and diffusion of lithium and sodium on defective rhenium disulfide: A first principles study. *ACS applied materials & interfaces* **2018,** *10* (6), 5373-5384.

[J18] Kavalsky, L.; Mukherjee, S.; Singh, C. V., Phosphorene as a Catalyst for Highly Efficient Nonaqueous Li–Air Batteries. *ACS applied materials & interfaces* **2018,** *11* (1), 499-510.

[J19] Haldar, S.; Mukherjee, S.; Singh, C. V., Hydrogen storage in Li, Na and Ca decorated and defective

borophene: a first principles study. *RSC advances* **2018,** *8* (37), 20748-20757.

[J20] Grixti, S.; Mukherjee, S.; Singh, C. V., Two-dimensional boron as an impressive lithium-sulphur battery cathode material. *Energy Storage Materials* **2018,** *13*, 80-87.

[J21] Cui, T.; Mukherjee, S.; Cao, C.; Sudeep, P. M.; Tam, J.; Ajayan, P. M.; Singh, C. V.; Sun, Y.; Filleter, T., Effect of lattice stacking orientation and local thickness variation on the mechanical behavior of few layer graphene oxide. *Carbon* **2018,** *136*, 168-175.

[J22] Cao, C.; Mukherjee, S.; Howe, J. Y.; Perovic, D. D.; Sun, Y.; Singh, C. V.; Filleter, T., Nonlinear fracture toughness measurement and crack propagation resistance of functionalized graphene multilayers. *Science advances* **2018,** *4* (4), eaao7202.

2017

[J23] Li, L.; Chen, L.; Mukherjee, S.; Gao, J.; Sun, H.; Liu, Z.; Ma, X.; Gupta, T.; Singh, C. V.; Ren, W., Phosphorene as a polysulfide immobilizer and catalyst in high-performance lithium–sulfur batteries. *Advanced Materials* **2017,** *29* (2), 1602734.

[J24] Haldar, S.; Mukherjee, S.; Ahmed, F.; Singh, C. V., A first principles study of hydrogen storage in lithium decorated defective phosphorene. *international journal of hydrogen energy* **2017,** *42* (36), 23018-23027.

[J25] Gao, A.; Mukherjee, S.; Srivastava, I.; Daly, M.; Singh, C. V., Atomistic Origins of Ductility Enhancement in Metal Oxide Coated Silicon Nanowires for Li-Ion Battery Anodes. *Advanced Materials Interfaces* **2017,** *4* (23), 1700920.

[J26] Cao, C.; Mukherjee, S.; Liu, J.; Wang, B.; Amirmaleki, M.; Lu, Z.; Howe, J. Y.; Perovic, D.; Sun, X.; Singh, C. V., Role of graphene in enhancing the mechanical properties of TiO_2/graphene heterostructures. *Nanoscale* **2017,** *9* (32), 11678-11684.

2016

[J27] Sun, H.; Mukherjee, S.; Singh, C. V., Mechanical properties of monolayer penta-graphene and phagraphene: a first-principles study. *Physical Chemistry Chemical Physics* **2016,** *18* (38), 26736-26742.

[J28] Sun, H.; Mukherjee, S.; Daly, M.; Krishnan, A.; Karigerasi, M. H.; Singh, C. V., New insights into the structure-nonlinear mechanical property relations for graphene allotropes. *Carbon* **2016,** *110*, 443-457.

[J29] Mukherjee, S.; Song, J.; Vengallatore, S., Atomistic simulations of material damping in amorphous silicon nanoresonators. *Modelling and Simulation in Materials Science and Engineering* **2016,** *24* (5), 055015.

2015

[J30] Nourmohammadi, Z.; Mukherjee, S.; Joshi, S.; Song, J.; Vengallatore, S., Methods for atomistic simulations of linear and nonlinear damping in nanomechanical resonators. *Journal of Microelectromechanical Systems* **2015,** *24* (5), 1462-1470.

2014

[J31] Keskar, N.; Mukherjee, S.; Krishna, K. M.; Srivastava, D.; Dey, G.; Pant, P.; Doherty, R.; Samajdar, I., Quantifying the mesoscopic shear strains in plane strain compressed polycrystalline zirconium. *Acta materialia* **2014,** *69*, 265-274.

CONFERENCE PRESENTATIONS

[C1] S. Mukherjee, C. V. Singh (2019) ,"Atomistic Simulations of Energy Dissipation in Amorphous Silica Nanoresonators", American Association for Advances in Functional Materials, Aug. 19-22, Los Angeles, USA.

[C2] C. Singh, T. Filleter, S. Mukherjee, "Nanomechanics of Graphene Oxide Nanosheets", American Association for Advances in Functional Materials, Aug. 19-22, Los Angeles, USA.

[C3] S. Barui, S. Mukherjee, K. Chattopadhyay (2019), "Data driven simulations for predicting phosphorus partition in BOF steelmaking", accepted for Presentation at 2019 International STEELSIM Conference, Aug. 13-15, Toronto, Canada.

[C4] S. Mukherjee, S. K. Mishra, I. Samajdar, P. Pant, "Local strain calculations using Electron Backscattered Diffraction (EBSD) measurements and digital image processing", Materials Science Forum, 702-703, ed: 2012, pp. 562-565.

INVITED ORAL TALKS

[T1] Molecular Dynamics Simulations of material Damping in silicon nanoresonators, Canada-India Collaboration in Nano Science & Technology, Edmonton, Alberta, Canada, May 5-10, 2013.

[T2] Machine learning for BOF steel making, Organized by AISTECH Mexico, Jan 24-25, 2019.

[T3] From Statistical Process Control (SPC) to Artificial Neural Networks (ANN) to Big Data to Machine Learning to Fundamental Assisted Analytics (FAA), University of South Alabama, USA, March 15, 2019.

[T4] Finite Element Simulations in Fracture Mechanics, Guest Lecturer at UofT, April 10, 2019

SERVICE & OUTREACH

Symposium organizer *(MS&T 2020, Pittsburgh, USA)*

"Mechanics of Materials for Energy Storage, Conservation, and Conversion"

Ad Hoc Reviewer

- *ACS Applied Materials & Interfaces* [Impact factor (2019)=8.46]
- *Carbon* [Impact factor (2019)=7.46]
- *Applied Surface Science* [Impact factor (2019)=5.16]
- *Journal of Physical Chemistry C* [Impact factor (2019)=4.3]
- *Physical Chemistry Chemical Physics* [Impact factor (2019)=3.56]
- *Chemical Physics Letters* [Impact factor (2019)=1.92]
- *Computational and Theoretical Chemistry* [Impact factor (2019)=1.34]