

## List of publications:

1. S. Mukherjee, L. Kavalsky, and C.V. Singh (2018), Ultrahigh storage and fast diffusion of Na and K in blue phosphorene anodes, *ACS Applied Materials & Interfaces*, 10 (10), 8630–8639
2. C. Cao\*, S. Mukherjee\*, J. Y. Howe, D. D. Perovic, Y. Sun, C. V. Singh, T. Filleter, Nonlinear fracture toughness measurement and crack propagation resistance of functionalized graphene multilayers. *Sci. Adv.* 4, eaao7202 (2018)
3. S. Mukherjee, J. Song, and S. Vengallatore (2016), Atomistic Simulations of Material Damping in Amorphous Silicon Nanoresonators, *MSMSE*, 2016
4. S. Mukherjee, A. Banwait, S. Grixti, N. Koratkar, and C.V. Singh (2018), Adsorption and diffusion of lithium and sodium on defective rhenium disulfide: A first principles study, *ACS Applied Materials & Interfaces*, 10(6), 5373–5384
5. Sun, H\*, Mukherjee\*, S, Krishnan, A, Manohar, KH, Daly, MA, and C.V. Singh (2016), New insights into structure-nonlinear mechanical property relations for graphene allotropes, *Carbon*.
6. Sun\*, H, Mukherjee\*, S, and C.V. Singh (2016), Mechanical properties of monolayer penta-graphene and phagraphene: a first-principles study, *Physical Chem Chem Phys*.
7. Z. Nourmohammadi\*, S. Mukherjee\*, S. Joshi, J. Song, and S. Vengallatore, Methods for Atomistic Simulations of Linear and Nonlinear Damping in Nanomechanical Resonators, *Journal of Microelectromechanical Systems*, 2015
8. Li, L, Chen, L, Mukherjee, S, Gao, J, Sun, H, Liu, Z, Ma, X, C.V. Singh, Ren, W, Cheng, HM, and Koratkar, N (2016), Phosphorene as a polysulfide immobilizer and catalyst in high-performance lithium-sulfur batteries, *Advanced Materials*.
9. C. Cao, Mukherjee, S., J. Liu, B. Wang, M. Amirmaleki, J. Y. Howe, D. Perovic, X. A. Sun, C.V. Singh, Y. Sun, T. Filleter (2017), Role of graphene in enhancing the mechanical properties of TiO<sub>2</sub>/graphene hetero-structures, *Nanoscale*, 9, 11678-11684
10. S. Grixti, S. Mukherjee, and C.V. Singh (2018), Two-dimensional boron as an impressive lithium-sulphur battery cathode material, *Energy Storage Materials*, 13, 80-87
11. N. Keskar, S. Mukherjee, K.V. Mani Krishna, D. Srivastava, G.K. Dey, P. Pant, R.D. Doherty, I. Samajdar, Quantifying the mesoscopic shear strains in plane strain compressed polycrystalline zirconium, *Acta Materialia*, vol. 69, pp. 265-274, 2014
12. T. Gao, S. Mukherjee, I. Srivastava, M. Daly, and C.V. Singh (2017), Atomistic Origins of Ductility Enhancement in Metal Oxide Coated Silicon Nanowires for Li-ion Battery Anodes, *Advanced Materials Interfaces*
13. S. Haldar, S. Mukherjee, F. Ahmed, and C.V. Singh (2017), A first principles study of hydrogen storage in lithium decorated defective phosphorene, *International Journal of Hydrogen Energy*, 42(36), 23018-23027
14. S. Mukherjee, S. K. Mishra, I. Samajdar, and P. Pant, Local strain calculations using Electron Backscattered Diffraction (EBSD) measurements and digital image processing, *Materials Science Forum* vol. 702-703, ed: 2012, pp. 562-565