- **Summit to: (Deep Learning and Modeling, Materials Discovery and Design)**

Theoretical Prediction and Characterization of Novel Two-Dimensional Ternary Tetradymite Compounds La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) as Anode Materials for Metal-Ion Batteries

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EXTENDED ABSTRACT:

Tetradymite compounds have triggered tremendous research interest from the scientific community because of their unique crystal structure and unprecedented properties. Herein, using state-of-the-art first-principles calculations, we identify that the La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) nanosheets exhibit structurally identical to Bi_2Te_2Se ternary teradymite type compounds with extraordinary electrical and electrochemical properties. It is first demonstrated that the layered La_2X_2Y compounds exhibit weak interlayer coupling with cleavage energy in the range of ~0.38-0.42 J/m^2, allowing ready separation of monolayers that can be synthesized through mechanical exfoliation from their bulk counterparts. Next, we comprehensively investigate the electrochemical properties of the predicted systems to evaluate their potential in metal-ion (Li/Na) batteries. Our detailed analysis reveals that the Li/Na adatom is sufficiently mobile on the surface of studied systems. For instance, the binding energy for Li(Na) on La_2GeI_2 is -2.24(-1.79) eV with a diffusion barrier of as small as ~0.31(0.20) eV. Subsequently, the maximum theoretical specific capacity for Li(Na) reaches as high as 887.0 (1364 mAg^{-1}), which can be attributed to a much higher storage capacity compared to previously identified 2D anode materials. Furthermore, we reveal that the predicted nanosheets exhibit a semiconducting nature and upon physically realistic strain, a Dirac cone can be realized, a striking finding that can be exploited in the transport properties. These findings substantiate that the predicted nanosheets could be synthesized to explore their potential applications in future metal-ion batteries.

Keywords: first-principles calculations, exfoliation, van der Waals tetradymite structure, Li/Na-ion battery, realization of Dirac cone under strain.

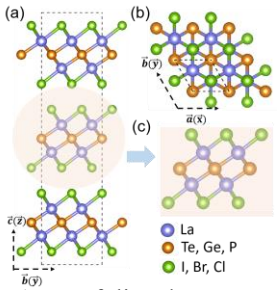

Figure1. Exfoliated La_2X_2Y (X = I, Br, Cl; Y = Ge, Te) nanosheets Tetradymite nanosheets.

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BIOGRAPHY

Nisar Muhammad is a Ph.D. student & an early stage researcher at the Hefei National Research Center for Physical Sciences at the Microscale, Department of Physics, University of Science and Technology of China. He has published six papers in reputed journals, I am highly enthusiastic about designing new materials for green energy by utilizing my knowledge, research abilities, and skills for the better interest of my institutions and humanity.