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Pore Formation in Graphene Oxide (GO): A First-Principles Study

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Abstract: Graphene oxide (GO) is an attractive material both as a scalable route for the mass production of graphene and for its own tunable electronic properties. The formation of nanopores during the oxidation of graphene has been reported, and porous GO has shown potential for various applications, including nanofiltration membranes. However, the random distribution of oxygen-containing functional groups in porous GO poses challenges to the reproducibility and specificity of its properties. In this work, we discuss the mechanism of pore formation in GO based on results from first-principles Density Functional Theory (DFT) calculations, which may help identify improved synthesis approaches for controlled porous GO structures.

Biography: Manuka Sinharage completed his Bachelor's degree in Physics from the University of Colombo in Sri Lanka. Manuka then earned his Master's in Physics from Southern Illinois University Carbondale, and he is currently a PhD student here at SIUC. His research focuses on computational materials physics and biophysics, where he uses computational methods to study the structural and electronic properties of advanced materials and biological systems.