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Theoretical investigation on 2D materials: Graphene, silicene, germanene and stanene

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Silicene, germanene, and tin; the 2D analogues of graphene are structurally different from graphene due to the buckling distortions in the lattice. Hybridization in graphene is purely sp<sup>2</sup>. It is sp<sup>2</sup>/sp<sup>3</sup> mixed orbitals in other 2D structures that results in buckling and causes pronounced effects in their properties. Structural, electronic, optical and mechanical properties are investigated. Density functional theory with generalized gradient approximation as implemented in CASTEP is used. At the Dirac point, the dispersion curve is linear in graphene and quadratic in all other materials. Critical points, saddle points, Van Hove singularities are investigated in band structures and density of states histograms. Optical properties unveil the frequency dependence and non-linear response of absorption. Graphene exhibits prominent absorption in the ultraviolet region and shifts towards the infrared region in all other 2D structures. Intensity of absorption increases in layered structures. Birefringence is exhibited by single and layered structures. Real part of refractive index establishes the anisotropic behavior. Bilayer exhibits semi-metallic behavior. Tri-layer portrays metallic nature. Study on mechanical properties brings out the unique stiffness of graphene. Bonding characteristics and charge density contours endorse that covalency reduces from graphene to stanene, due to which elastic moduli decreases from graphene to stanene. Poisson's ratio shows increased brittleness in graphene, semi-metallic nature in silicene and germanene, and metallic nature in stanene. Although, silicene, germanene and stanene possess only 20%, 14%, and 9% of Young's modulus, respectively, the bonding nature facilitates its suitability in semiconductor industry along with substrates to enhance the conduction mechanism.

## Biography

Rita John is a Professor and Head, Department of Theoretical Physics, University of Madras, Chennai, India. She is a Visiting Professor at the Department of Physics and Astronomy, Texas Christian University, Fort Worth, Texas, USA (2014). She has been teaching Solid State Physics for graduate students over 18 years. The book, *"Solid State Physics"* is authored by her and published by Tata McGraw Hill publisher (2014) is used globally by graduate students. She has over 50 international publications. She is the recipient of various awards and prizes for her academic and research contributions.

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