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**Electronic and optical properties of ultrathin silicon nanomembranes: A first-principles investigation** WOOSUN JANG, SU-HYUN YOO, ALOYSIUS SOON, Global E3 Institute and Department of Materials Science and Engineering, Yonsei University, Seoul 120-749, Korea — Owing to its unique and exotic physical and chemical properties, there has been a lot of effort undertaken to explore and study ultrathin low-dimensional nanostructures (e.g. graphene and MoS2). Of late, two-dimensional (2D) nanomembranes of silicon - a well-known prototypical bulk semiconductor - have attracted much attention, and has found its potential in niche nanodevice applications e.g. field effect transistors (FET) and secondary battery anodes. In this work, after considering various nanomembranes of Si with varying thicknesses, we study geometric and electronic structures using first-principles density-functional theory calculations (and beyond). Here, we consider both bulk-terminated pristine Si nanomembranes as well as surface-reconstructed ones, as motivated by available experimental and theoretical reports. To understand the influence of growth conditions on these Si nanomembranes, we have also studied the role of surface-passivation (e.g. with O, H, and OH) on their electronic and optical properties. Namely, we carefully investigate their thickness-dependent electronic band structure (i.e. both their fundamental and optical band gap energies), so as to elucidate their intrinsic structure-property relations for designing future technologically important nanodevices.

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