How does Goldene Stack?

Marcelo Lopes Pereira, Jr[1], Emanuel J. A. dos Santos [2], Luiz Antonio Ribeiro, Jr[2] and Douglas Soares Galvão.[3]

University of Brasília, College of Technology, Department of Electrical Engineering, Brasília, Federal District, Brazil.[1]
Institute of Physics, University of Brasília, 70910-900, Brasília, Brazil.[2]
Department of Applied Physics and Center for Computational Engineering and Sciences, State University of Campinas, Campinas, São Paulo, Brazil.[3]

The article investigates the structural and electronic behavior of Goldene, a recently synthesized atomic gold monolayer, as it stacks into multiple layers, eventually transitioning to the bulk phase. Using density functional theory (DFT) calculations, the researchers observed that Goldene maintains an AA-type stacking up to six layers, without exhibiting the Bernal (AB) configuration commonly seen in other 2D materials, such as graphene. Starting from seven layers, a spontaneous transition occurs to a bulk-like rhombohedral (ABC) structure, typical of face-centered cubic (FCC) gold. At ten or more layers, the convergent structure fully aligns with the bulk phase. Quantum confinement effects play a central role in Goldene's electronic properties. While the monolayer and bulk gold share a single Dirac cone at the X-point of the Brillouin zone, multilayer systems display two Dirac cones at the X and Y points. The study shows that Goldene's stacking affects the positioning of these cones and contributes to anisotropic electronic transport. Furthermore, the monolayer exhibits significant anisotropic optical absorption in the UV-visible spectrum, particularly when light is polarized along the in-plane directions (x and y). This characteristic disappears as the system transitions to the bulk phase, resulting in more isotropic and less intense optical absorption. Phonon calculations indicate that Goldene is structurally stable in both its monolayer and multilayer forms. The absence of imaginary frequencies in the phonon dispersion curves confirms its dynamic stability, which is essential for practical applications. Mechanical stability is further supported by consistent cohesive energies and minor increases in bond lengths as the layers stack. The study also highlights that Goldene's stacking behavior is distinct from that of graphene, where Bernal stacking dominates. In Goldene, weak interlayer interactions, driven by van der Waals forces, preserve many of the monolayer's electronic features even in systems with up to six layers. However, as stacking progresses beyond seven layers, interlayer interactions become significant, causing structural and electronic changes that converge toward the bulk state. These findings underscore the importance of controlling Goldene's stacking, enabling tunability of its electronic and optical properties. The practical implications include designing optoelectronic devices and exploring new functionalities in metallic 2D materials.

Keywords: Goldene, Multilayered Goldene, Structural Transitions, Quantum Confinement, DFT

References

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