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Ab initio Calculations of Geometric and Electronic Structure of Graphene-Au System ROBERTO NUNEZ-GONZALEZ, Dept. de Matemáticas, Universidad de Sonora, DONALD H. GALVAN, Centro de Nanociencias y Nanotecnología,Unam, ALVARO POSADA-AMARILLAS, Dept. de Inv. en Física, Unison — Structural and electronic properties of graphene with one gold atom at top were calculated using the Full-Potential Augmented Plane Waves with Local Orbitals Method and the local density approximation (LDA), within the Density Functional Theory. For the calculations, we use a 3x3x1 supercell of graphene, calculating the stability of the system with the gold atom at three different sites: Hole, Bridge and Top sites. For each site, the atoms are relaxed minimizing forces. An analysis of the structural properties is performed for each site, calculating the density of states (DOS). A comparison with pure graphene is realized.

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