Supporting Information for the article

“Electronic Structure of Atomically Precise Graphene Nanoribbons” by

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Interaction between 7-AGNR and Au(111)

To characterize the adsorption of 7-AGNRs on Au(111), we have performed first-principles calculations at the DFT-LDA level of theory. We used a Au(111) slab with 5 layers on top of which the 7-AGNR has been adsorbed. A vacuum region of 12 Å has been included. The gold slab was passivated by hydrogen on one side to inhibit interaction among Au(111) surface states. For comparison with established results for graphene (Gr) on Au(111) [1], we performed the same calculations also for Gr/Au(111). We find a Gr/Au distance of 3.31 Å and a negligible electronic interaction (i.e. band hybridization), in excellent agreement with the findings of Ref. [1]. For the H-passivated 7-AGNR we determine an average C-Au distance of 3.15 Å, and little to negligible band hybridization of the electronic bands of GNRs and Au(111) (Fig. S1). This clearly shows that the interaction between 7-AGNR and the Au(111) metal substrate is weak. The electronic structure of the 7-AGNR is essentially preserved in this weak binding “physisorption” regime.

Our experimental findings are fully compatible with a weak “physisorption” interaction between GNRs and the Au(111) substrate. On the one hand, we find no sign of partially filled bands or bands populated/depopped upon adsorption. On the other hand, the ARPES data given in Figs. 3 and 4 of the manuscript show an unperturbed valence band dispersion (parabolic top, linear at lower energies), which would not be expected for a strongly interacting system.

[1] Khomyakov et al., Phys Rev B 79, 195425 (2009).

Figure S1: Band structure and density of states (DOS) of the 7-AGNR adsorbed on Au(111) from DFT-LDA calculations. The Fermi energy of the hybrid system is set to zero. The band structure of the hybrid system 7-AGNR/Au(111) is shown by grey lines. Black lines correspond to the band structure / DOS of the isolated ribbon computed at frozen adsorption geometry. Red dots correspond to the projection amplitude of the Kohn-Sham orbitals of the whole system onto atomic orbitals of the nanoribbon. Larger dots indicate a larger projection amplitude (ranging from 0 to 1 by definition). The dot scale ranges from 5% to 50% in the figure, indicating a projection amplitude of at least the given value. Red lines correspond to the DOS obtained from the projection.