Supporting Information

Ultranarrow heterojunctions of armchair-graphene nanoribbons as resonant-tunneling devices

F. Sánchez-Ochoa[*a], Jie Zhang[b], Yueyao Du[b], Zhiwei Huang[b], G. Canto[c], Michael Springborg[d] and Gregorio H. Cocoletzi[e]

[a]*Universidad Nacional Autónoma de México, Instituto de Física, Apartado Postal 20-364, Cd. de México 01000, Mexico*
[b]*Department of Environmental Science & Engineering, Huaqiao University, Xiamen 361021, People's Republic of China*
[c]*Centro de Investigación en Corrosión, Universidad Autónoma de Campeche, Av. Héroe de Nacozari 480, 24079 Campeche, Campeche, Mexico*
[d]*Physical and Theoretical Chemistry, University of Saarland, 66123 Saarbrücken, Germany*
[e]*Benemérita Universidad Autónoma de Puebla, Instituto de Física, Apartado Postal J-48, Puebla 72570, Mexico*

To whom correspondence should be addressed Email: fsanchez@fisica.unam.mx; franciscosno88@gmail.com

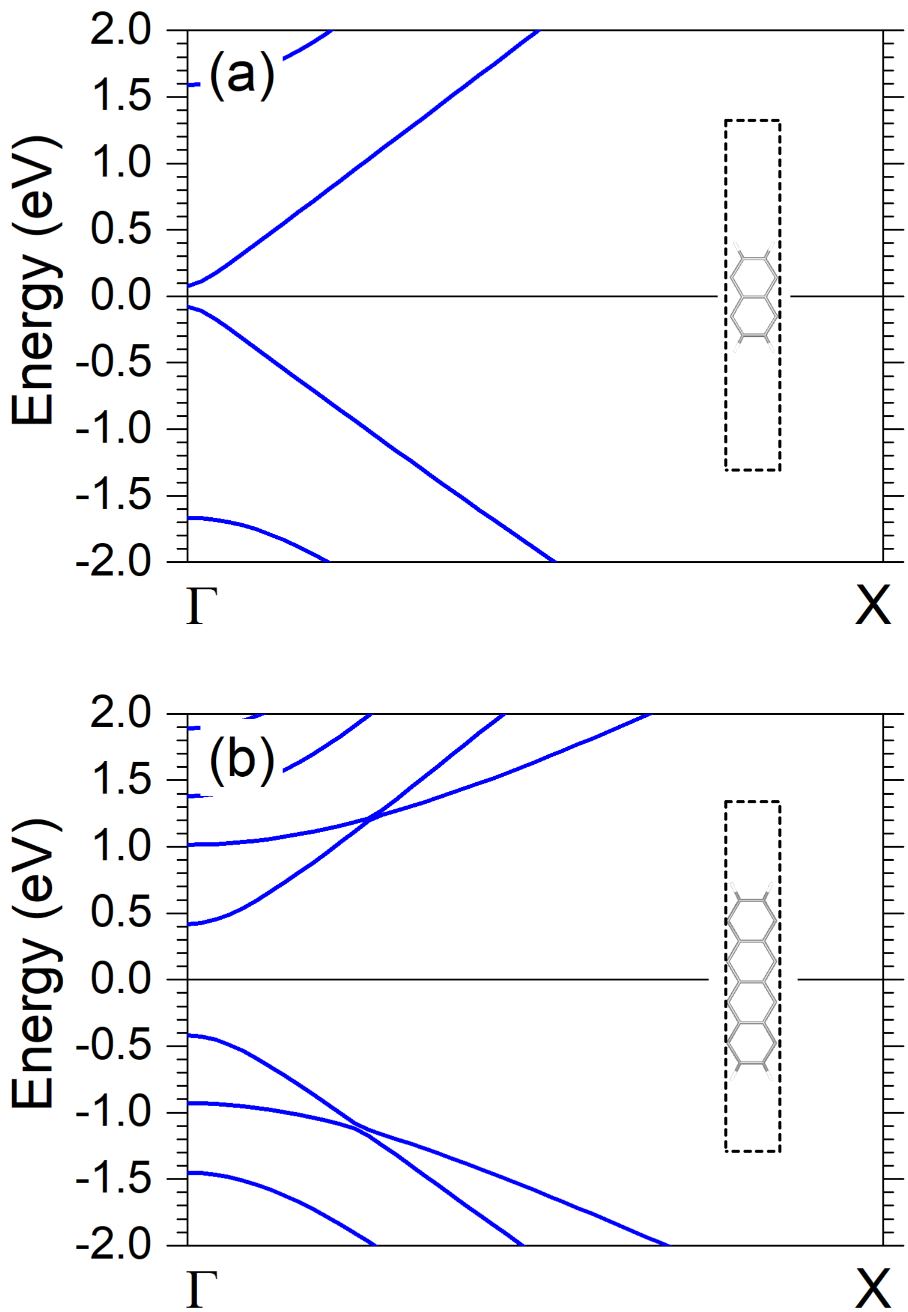

Figure S1. Calculated electronic band structures of periodic and infinite armchair graphene nanoribbons with (a) five dimers and (b) nine dimers as width. Band gaps are present in both band structures. The Fermi level is set to 0 eV. The insets show the elementary unit cells of (a) 5-AGNR and (b) 9-AGNR systems with gray and white sticks representing C and H atoms, respectively.

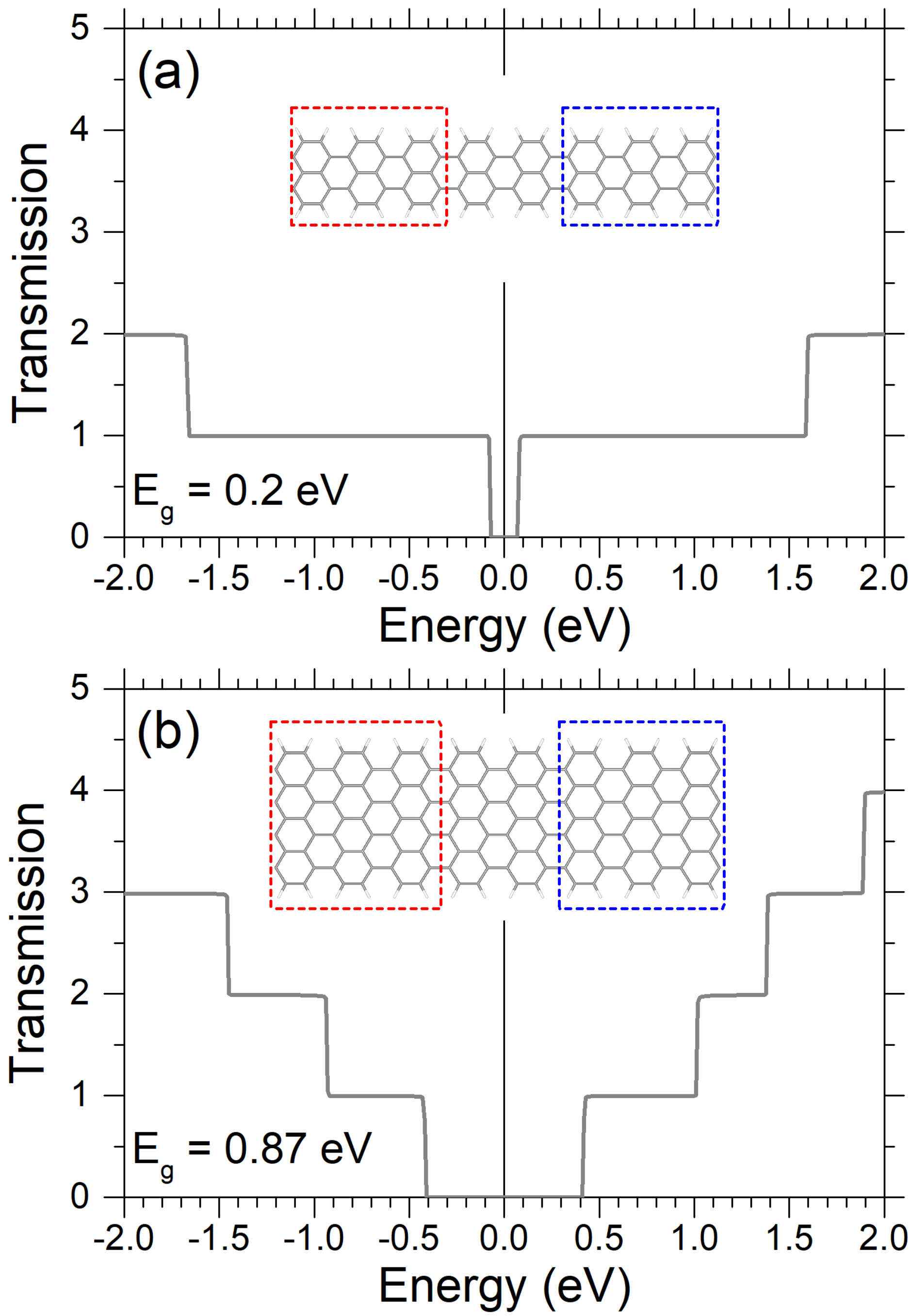

Figure S2. Spin-up electronic transmission as function of electron energy for two ideal nanoribbons at equilibrium conditions. (a) 5-AGNR and (b) 9-AGNR. Narrow band gaps are present in both transmission plots as those in electronic band structures. The insets show the ideal (a) 5-AGNR and (b) 9-AGNR devices, with left- and right-lead enclosed by red- and blue-dashed rectangles, respectively. The Fermi level is set to 0 eV.

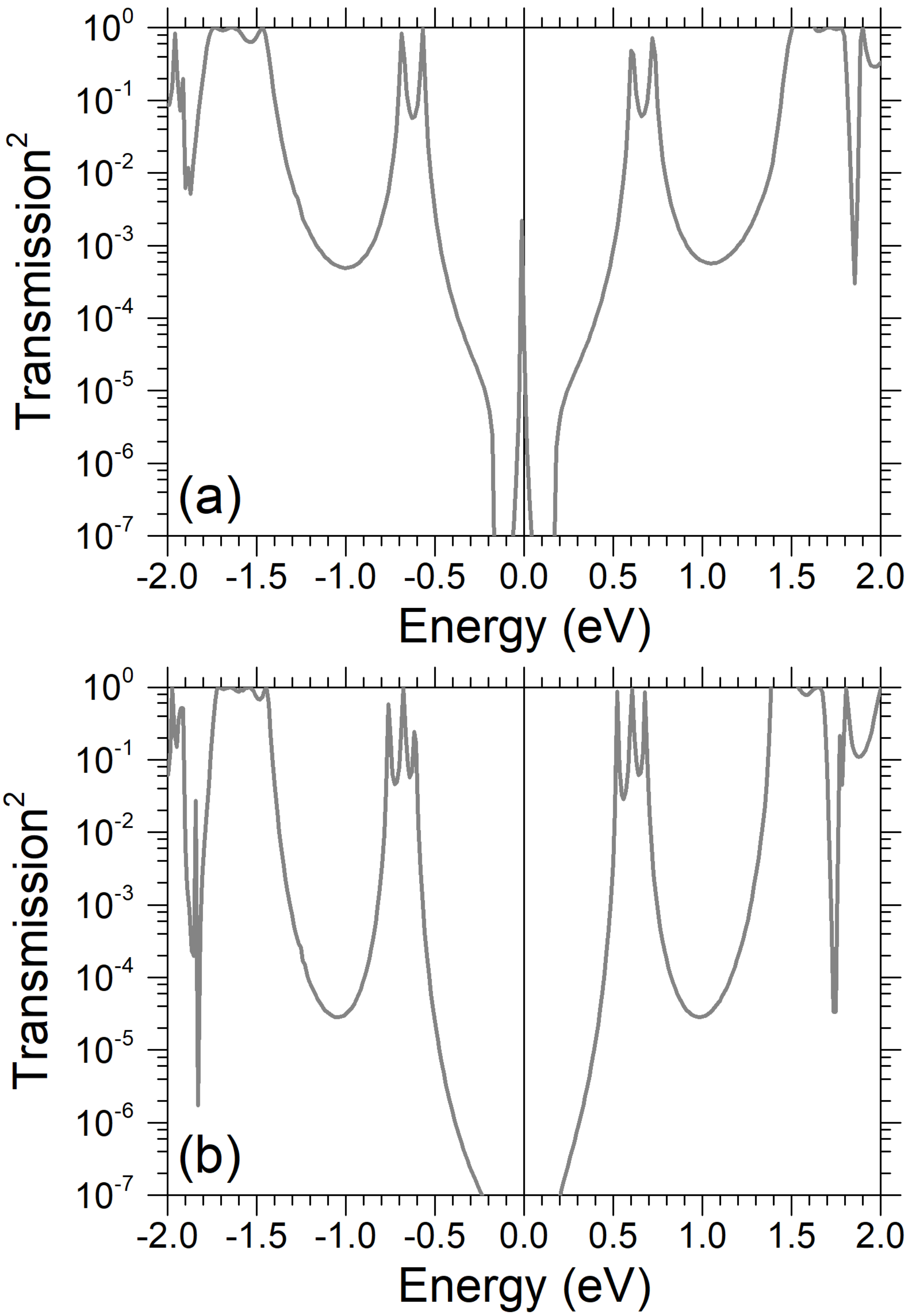

Figure S3. Log-scale square electronic transmission for spin-up states as function of electron energy for two devices with (a) three barriers (2 wells) and (b) four barriers (3 wells) at equilibrium conditions. The energy band splitting is observed in the first electronic resonance at ~±0.6 eV in valence and conduction bands. The Fermi level is set to 0 eV.

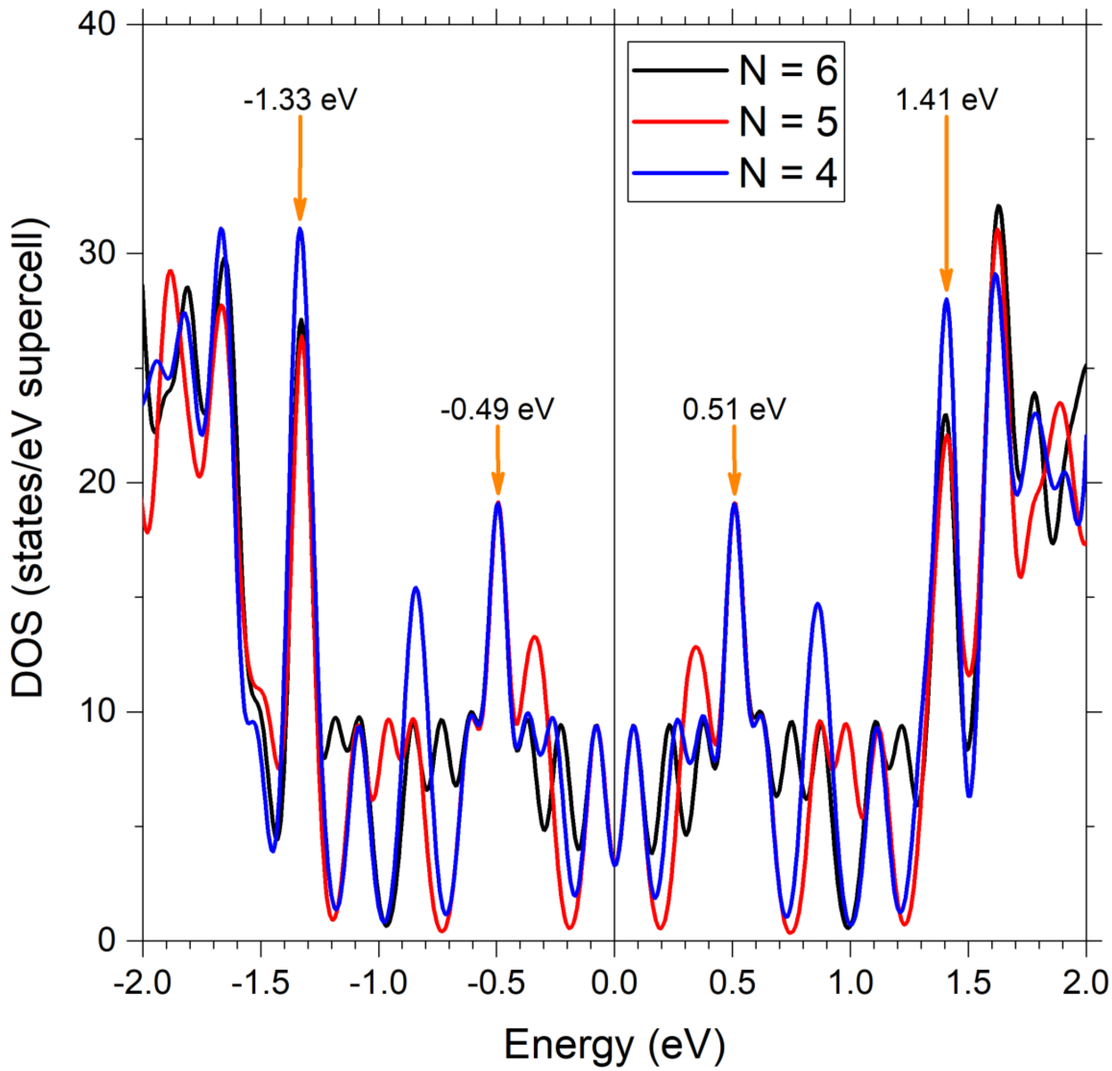

Figure S4. Calculated electronic density of states (DOS) for the whole device, scattering region plus left and right leads and buffer atoms by means of self-consistent DFT calculations with standard diagonalization method in SIESTA. N represents the number of 5-AGNR units in the quantum well. Orange arrows indicate localized states. Only spin-up states contributions are plotted. The Fermi level is set to 0 eV.

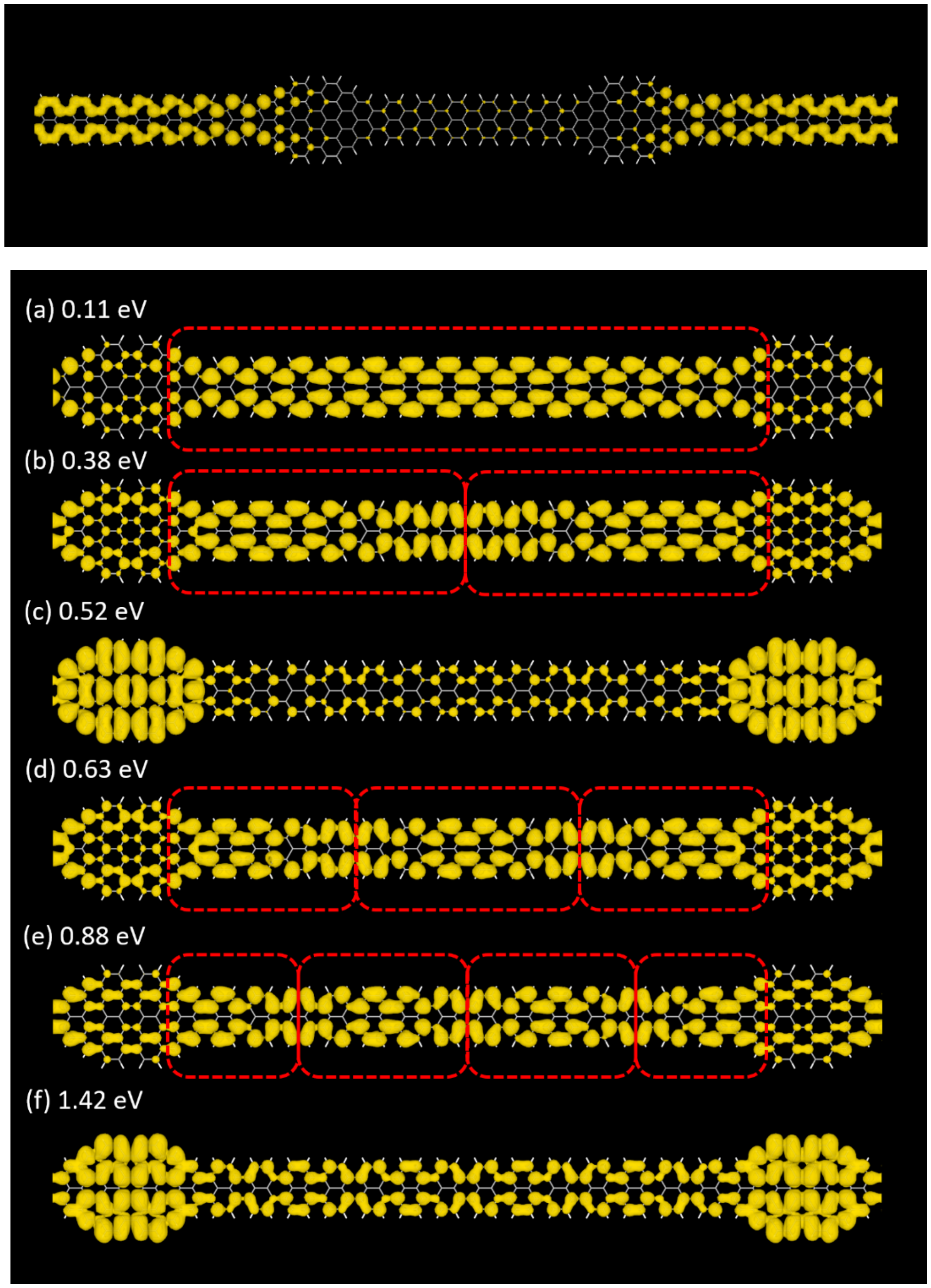

Figure S5. Calculated local density of states (LDOS) maps. Top panel: LDOS calculated at the Fermi level, or zero eV in transmission plots, for the device with six 5-AGNR units forming the well. Bottom panel: The device with fourteen 5-AGNR units in the quantum well showing in (a), (b), (d) and (e) the first four resonances above the Fermi level, while (c) and (f) are first two localized states. For the integration of electronic states in LDOS, the window energy was 40 meV. The isosurface value was 7.96×10^{-5} e/Å^3. The dashed-red lines show quantized states for n=1-4, each with n lobes and n-1 nodes. Bound states and localized states show a weak admixture from each other.

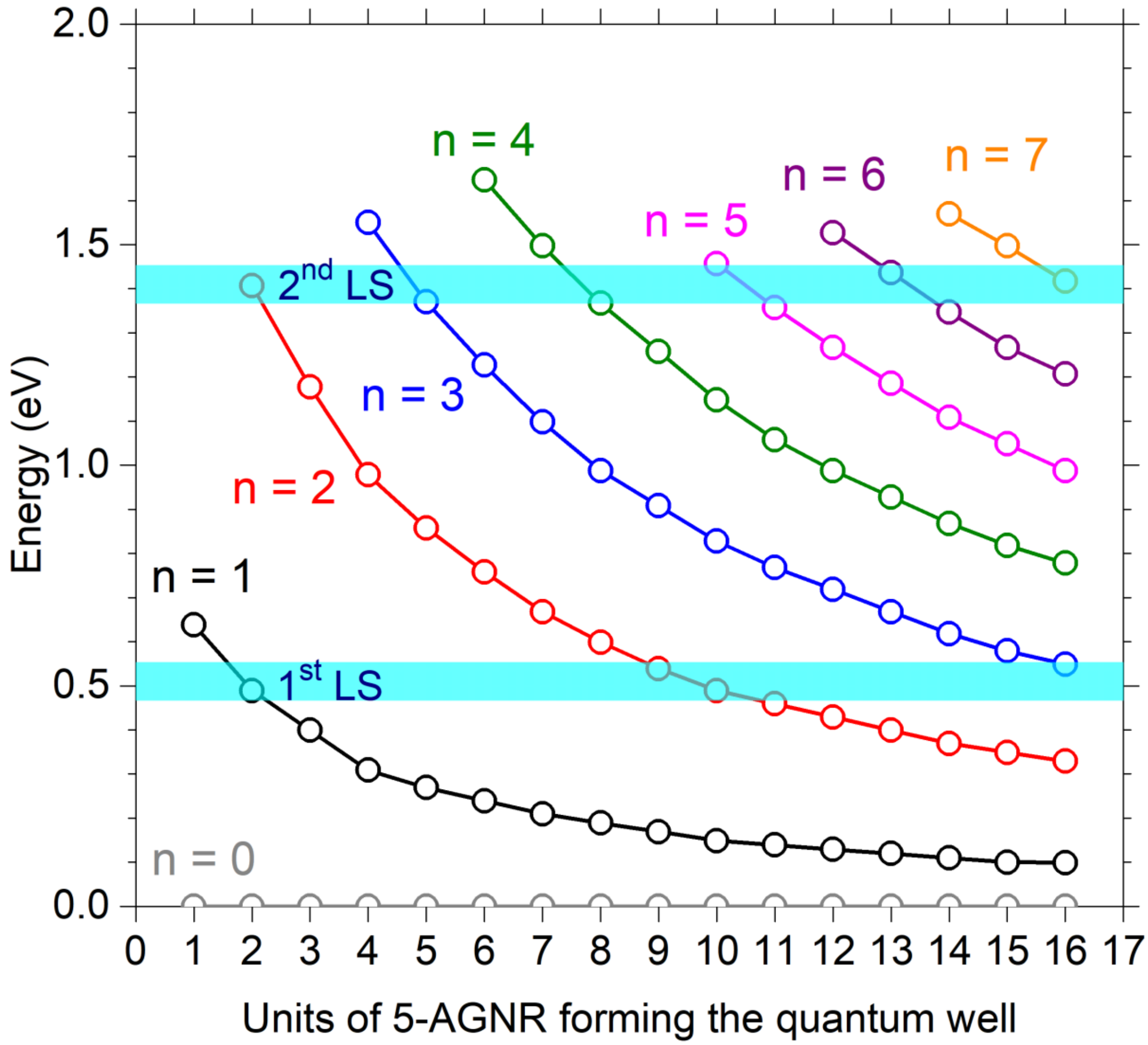

Figure S6. Electronic resonances as function of energy and width of quantum well. First eight resonances, *n*=0-7, are shown for the unoccupied states. Horizontal cyan bars highlight the positions of 1st and 2nd localized states (LS) in potential barriers built with 9-AGNR units. The resonance with *n*=0 eV is fixed at the Fermi level. The Fermi level is set to zero eV.

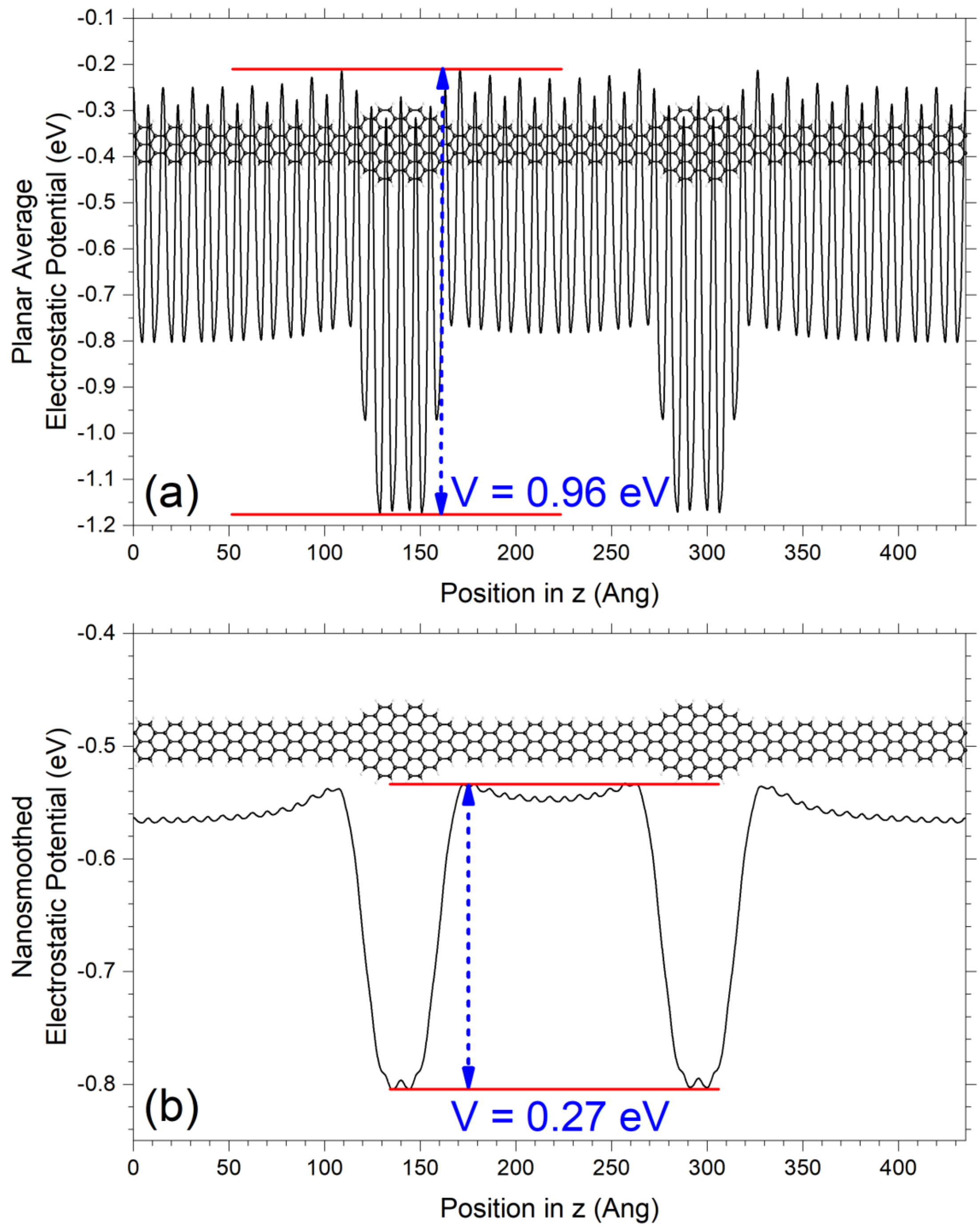

Figure S7. Top panel: Planar electrostatic potential along the transport (z) direction for sixth device. Bottom panel: Average (nanosmothed) electrostatic potential calculated from top panel. As can be seen, two potential barriers form a quantum well for occupied states. A symmetric potential is generated for unoccupied states.

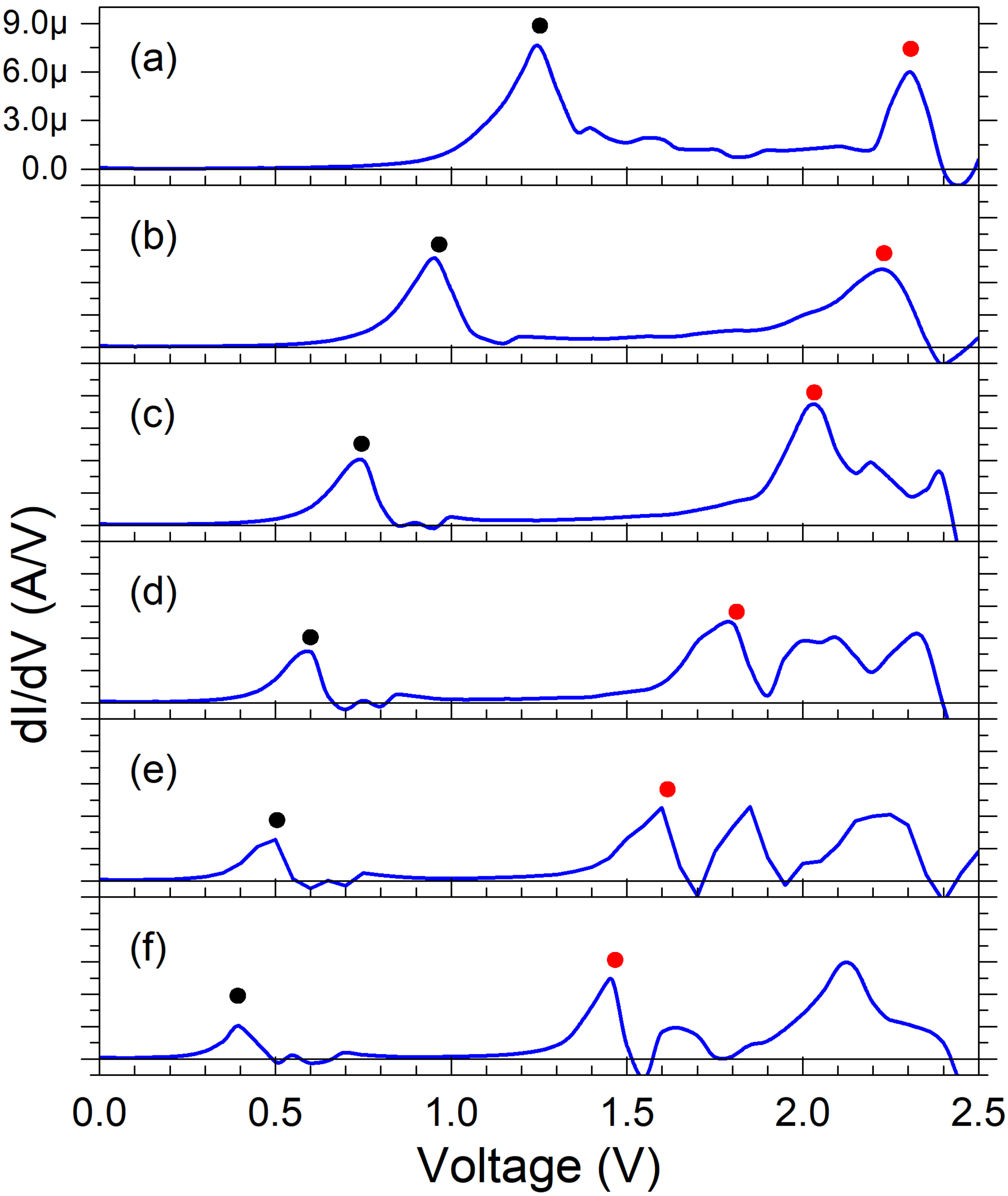

Figure S8. Calculated differential conductance of spin-up unoccupied states for devices with (a) one to (f) six 5-AGNR units within the well. Black and red points represent the first and second resonances moving towards 0 V as the width of quantum well increases.

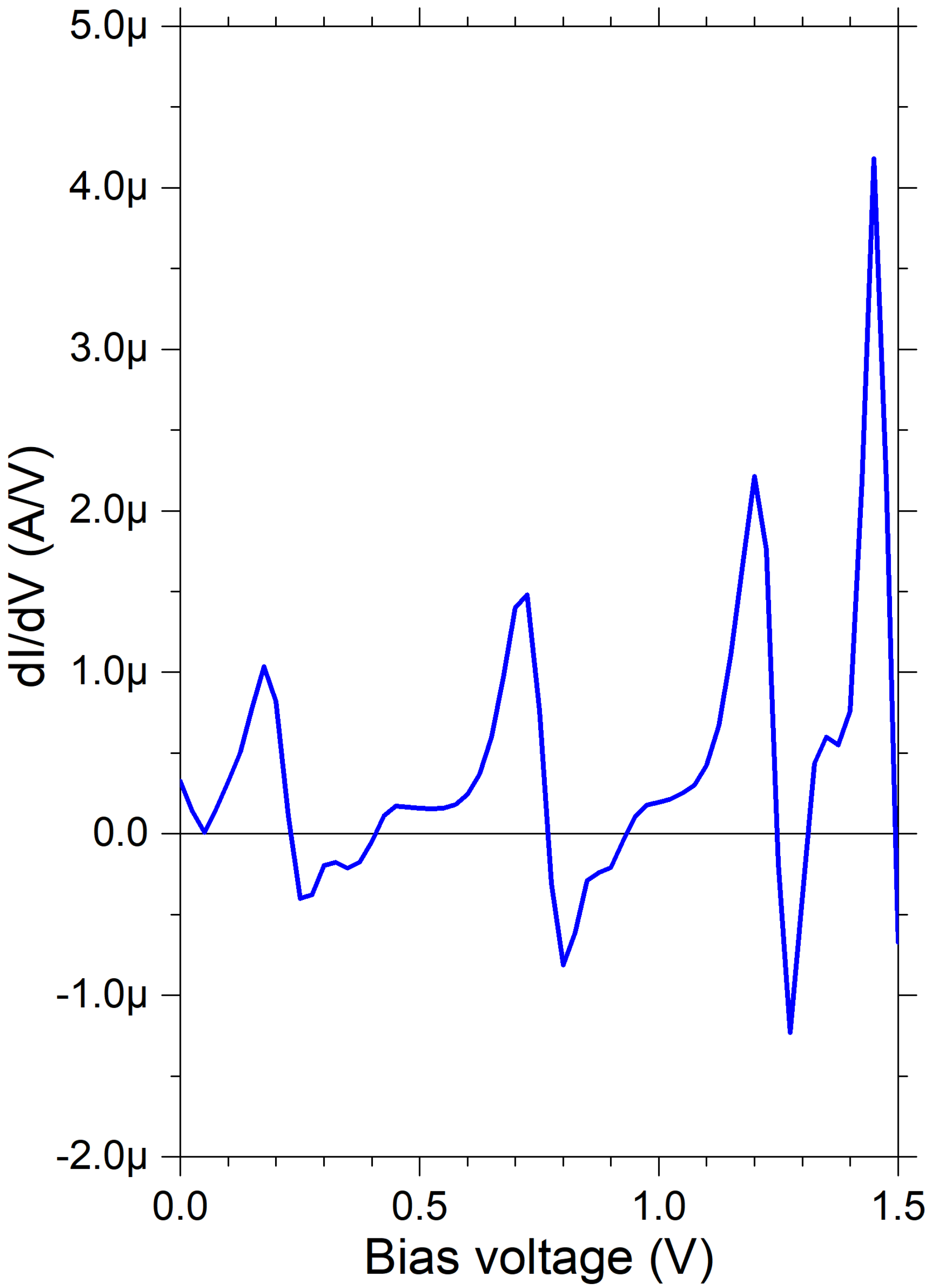

Figure S9. Calculated spin-up differential curve (dI/dV) for device with fourteen 5-GNR within well. dI/dV shows negative regions of differential conductance with promising applications as tunnel devices.