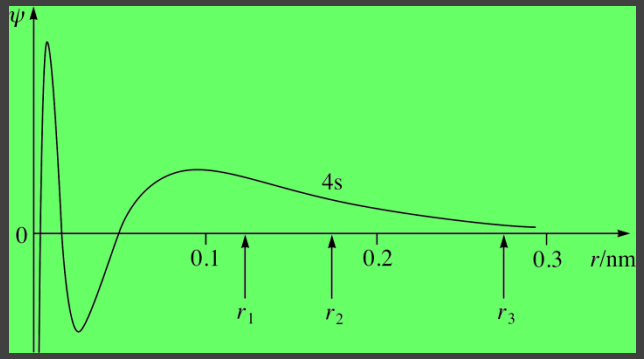
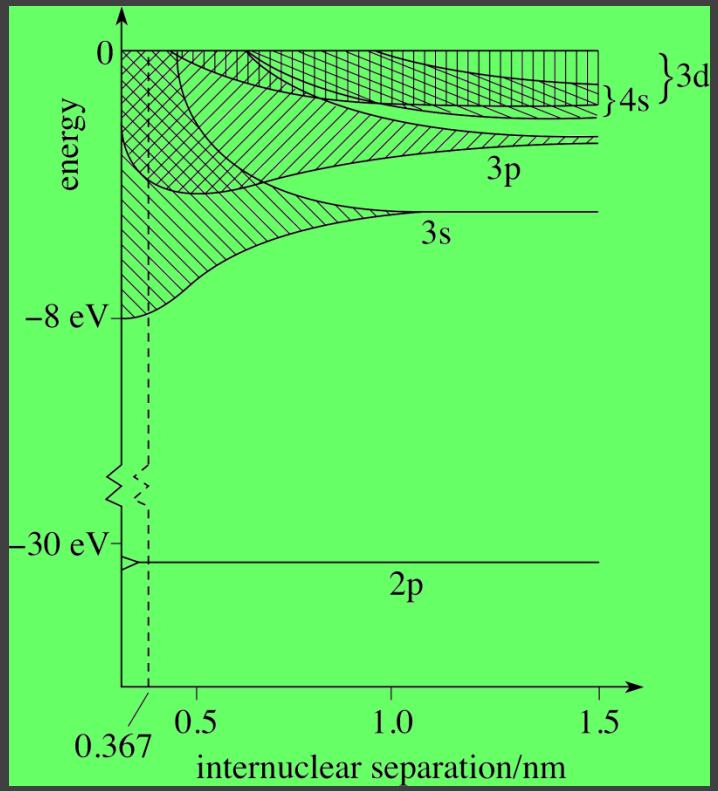
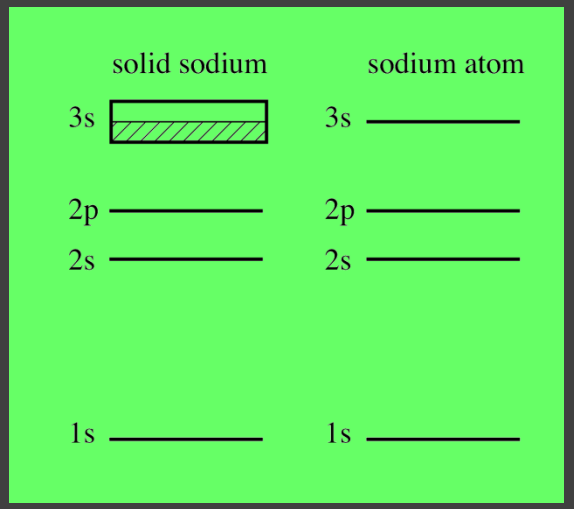


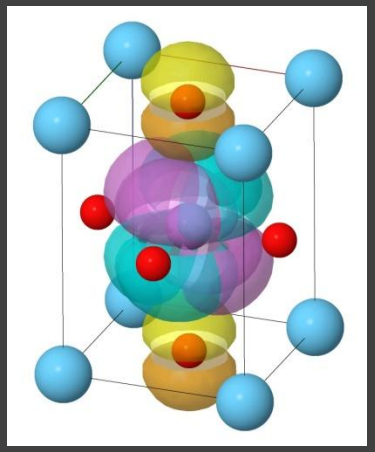
Funcion de onda 4s de un atomo de Ni,
indicacion primeros, segundos y terceros vecinos
Ni [Ar] $3d^8\ 4s^2$

Na

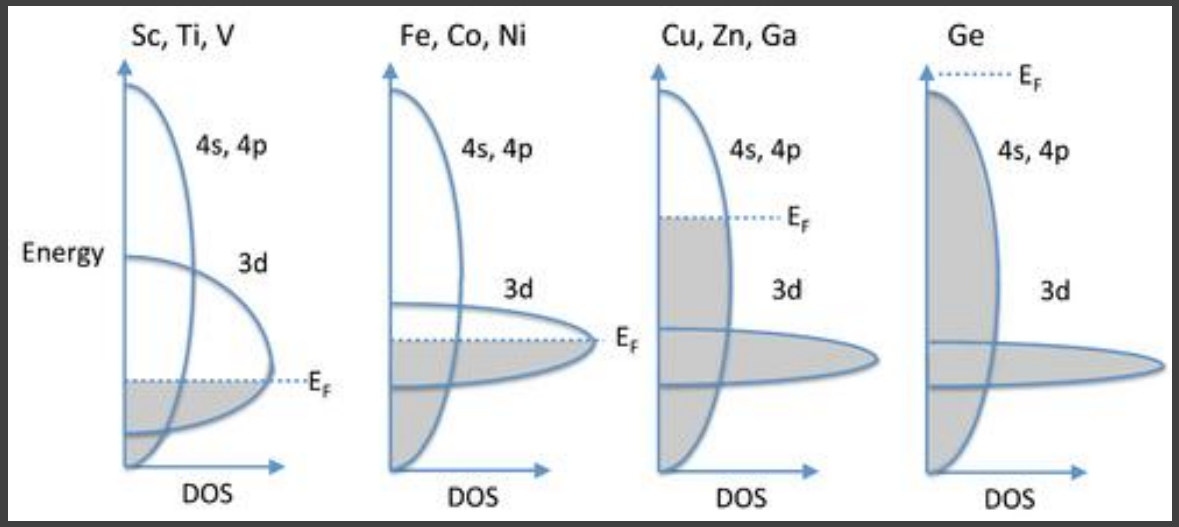
$1s^2\ 2s^2\ 2p^6\ 3s^1$







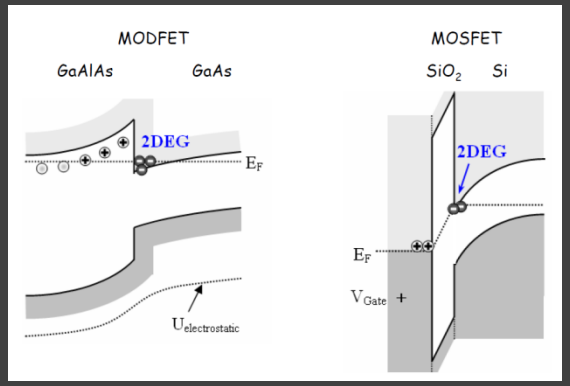
ABO_3

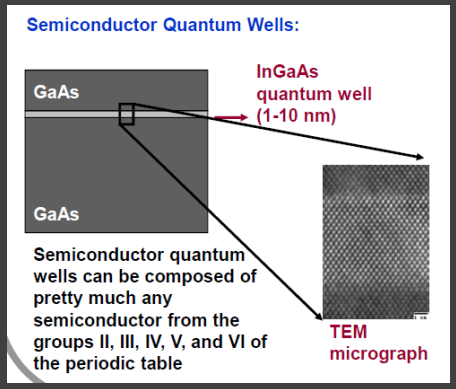


Gases de electrones 2D

Tipicamente en interfaces semiconductores

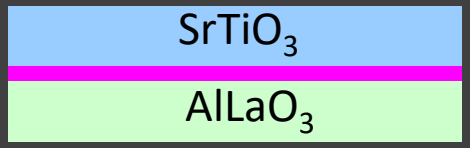
GaAs/ Al GaAs





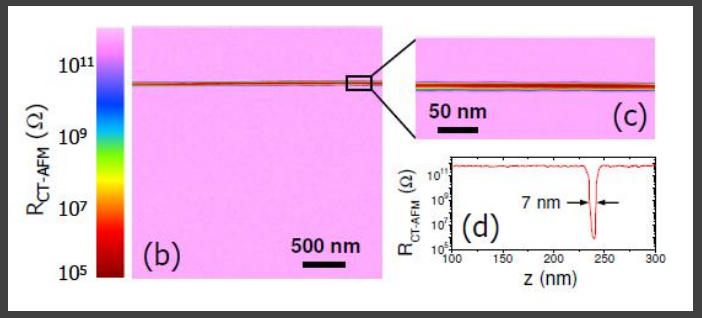
Recientemente:

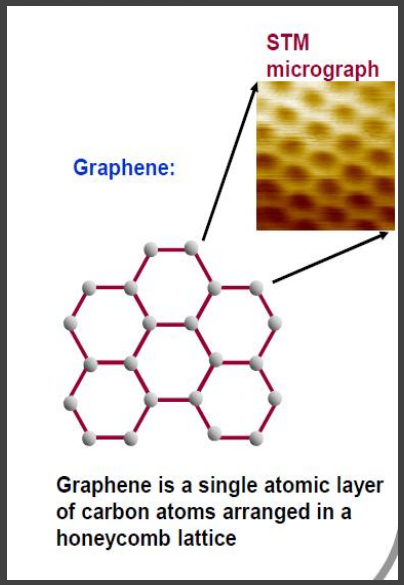
2010



GAS 2DEG

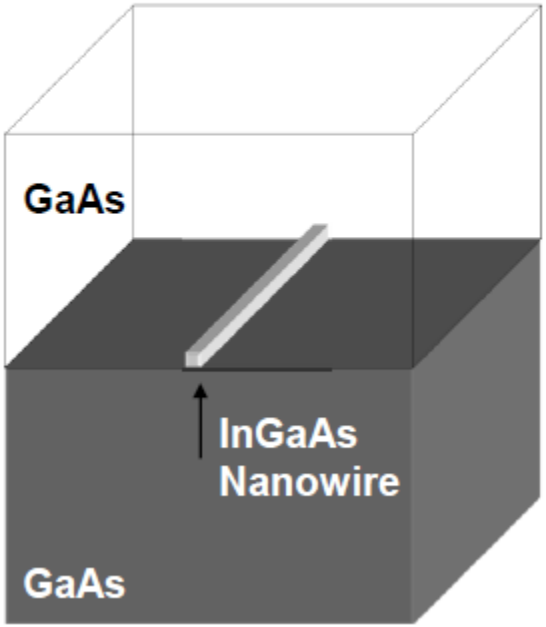
Metal!!



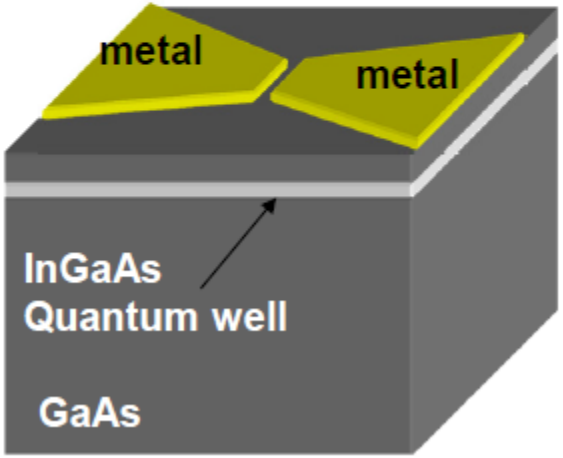


Gases de electrones 1D

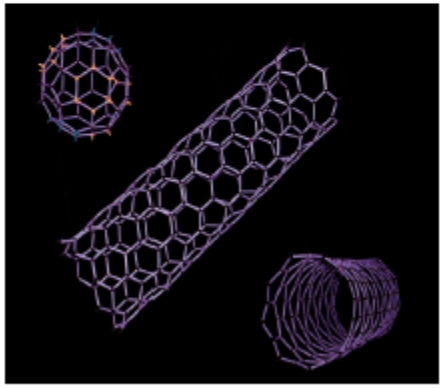
Semiconductor Quantum Wires (or Nanowires):

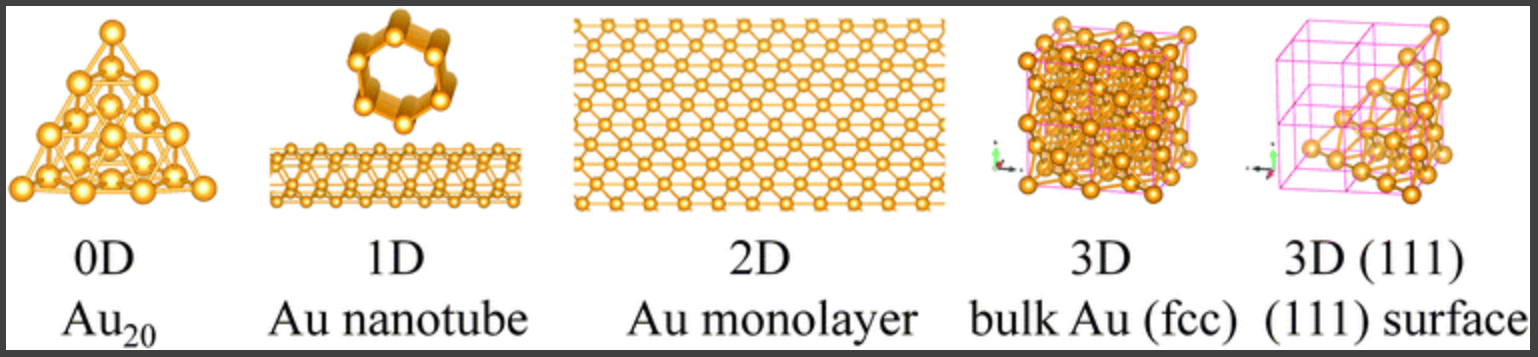


Semiconductor Quantum Point Contacts (Electrostatic Gating):



Carbon Nanotubes (Rolled Graphene Sheets):





MONOCAPA ORO

ORO BULK

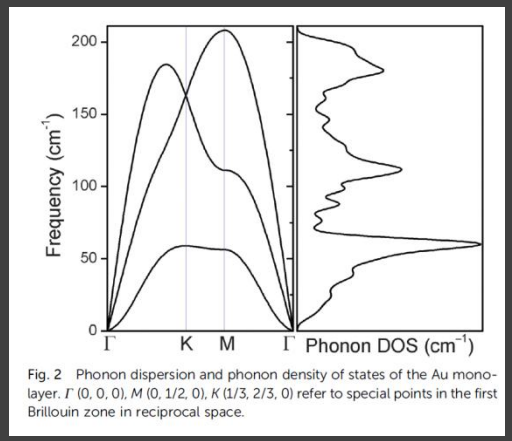


Fig. 2 Phonon dispersion and phonon density of states of the Au monolayer. Γ (0, 0, 0), M (0, 1/2, 0), K (1/3, 2/3, 0) refer to special points in the first Brillouin zone in reciprocal space.

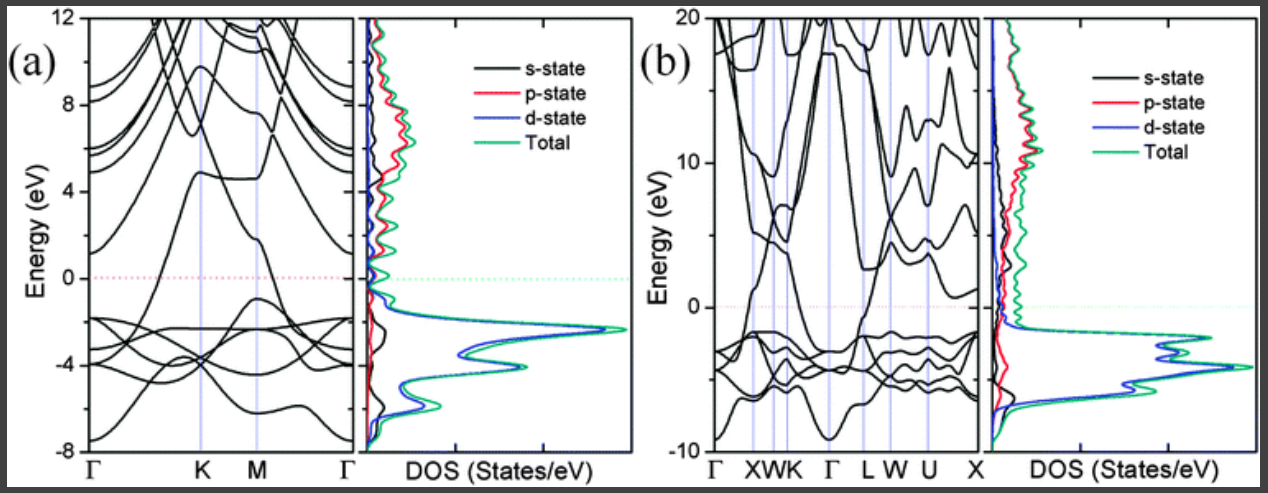


Fig. 4 Electronic structures of 2D Au monolayer (a) and 3D bulk Au (b). Band structure (left), total density of states (TDOS) and partial density of states (PDOS) (right) are shown. The Fermi level is at 0 eV.

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Quasi one-dimensional band dispersion and surface metallization in long-range ordered polymeric wires

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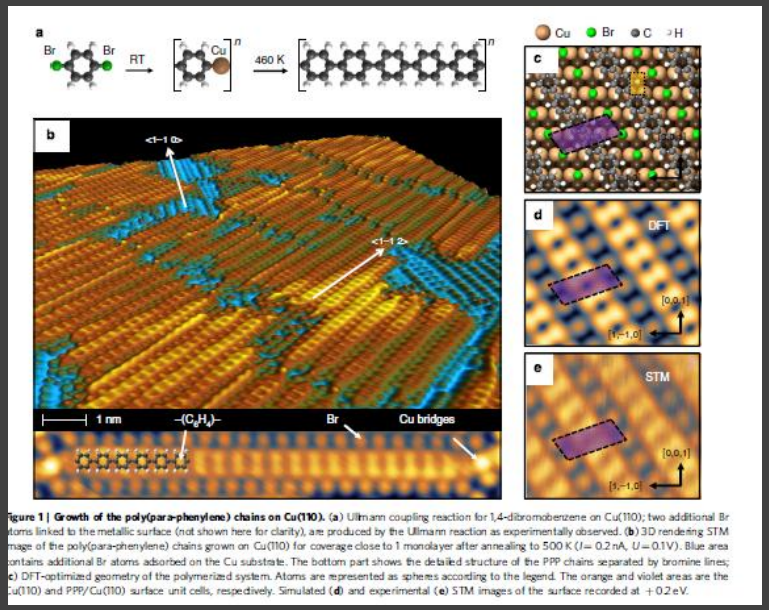


Figure 1 | Growth of the poly(para-phenylene) chains on Cu(110). (**a**) Ullmann coupling reaction for 1,4-dibromobenzene on Cu(110); two additional Br atoms linked to the metallic surface (not shown here for clarity), are produced by the Ullmann reaction as experimentally observed. (**b**) 3D rendering STM image of the poly(para-phenylene) chains grown on Cu(110) for coverage close to 1 monolayer after annealing to 500 K ($I = 0.2$ nA, $U = 0.1$ V). Blue area contains additional Br atoms adsorbed on the Cu substrate. The bottom part shows the detailed structure of the PPP chains separated by bromine lines; (**c**) DFT-optimized geometry of the polymerized system. Atoms are represented as spheres according to the legend. The orange and violet areas are the Cu(110) and PPP/Cu(110) surface unit cells, respectively. Simulated (**d**) and experimental (**e**) STM images of the surface recorded at +0.2 eV.

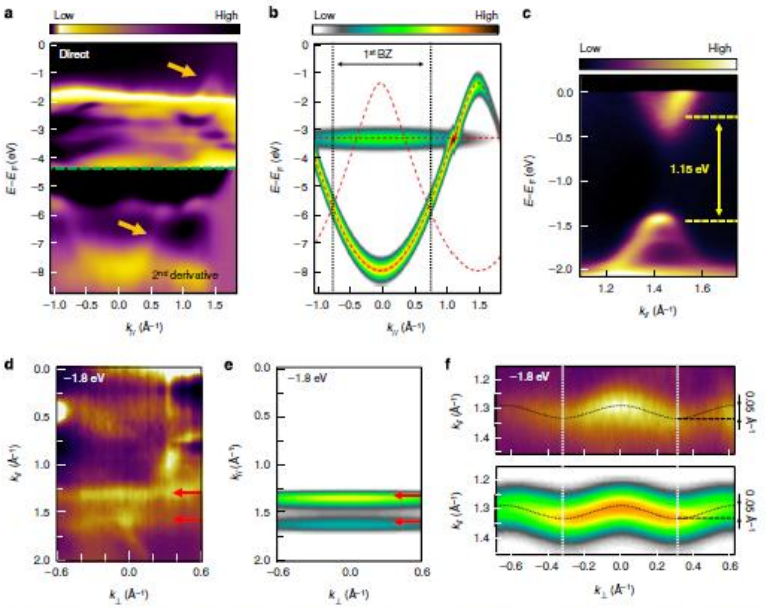


Figure 3 | Angle-resolved photoelectron spectroscopy measurements. (**a**) ARPES intensity map measured along the <1-12> direction, parallel to the polymers chains for 1ML-PPP/Cu(110). The bottom part is displayed in second derivative. Arrows indicate bands due to the presence of polymers. (**b**) Tight-binding modelling of the band structure of the $N = 20$ PPP polymer using $\beta = -3.5$ eV. (**c**) High-resolution ARPES intensity map recorded close to the Fermi level showing the HOMO–LUMO bandgap. Measurements (**d**) and tight-binding modelling (**e**) of the ARPES constant energy map at −1.8 eV. (**f**) Zoom on the measured (top) and calculated (bottom) ARPES constant energy maps. The transverse resonance integral used in the calculations is $\beta' = -0.15$ eV.

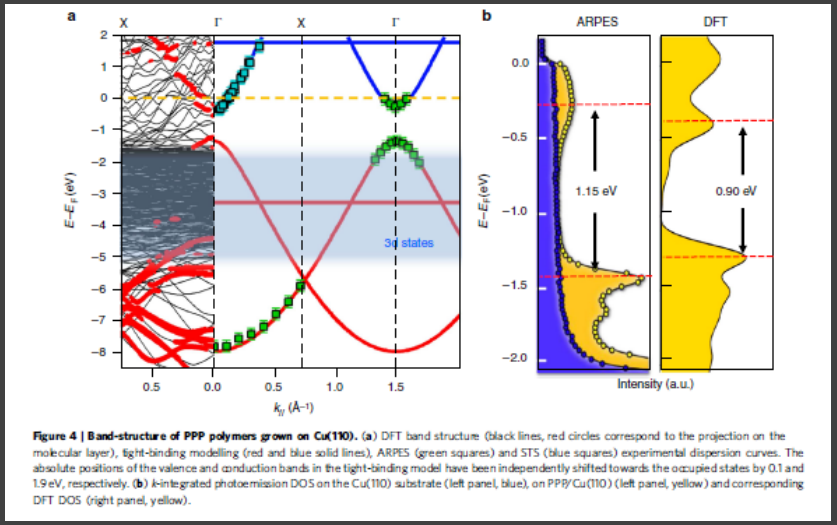


Figure 4 | Band-structure of PPP polymers grown on Cu(110). (**a**) DFT band structure (black lines, red circles correspond to the projection on the molecular layer), tight-binding modelling (red and blue solid lines), ARPES (green squares) and STS (blue squares) experimental dispersion curves. The absolute positions of the valence and conduction bands in the tight-binding model have been independently shifted towards the occupied states by 0.1 and 1.9 eV, respectively. (**b**) *k*-integrated photoemission DOS on the Cu(110) substrate (left panel, blue), on PPP/Cu(110) (left panel, yellow) and corresponding DFT DOS (right panel, yellow).

Relacion de dispersion, derecha densidad de estados de una monocapa, 1D-like

Efecto de sustratos

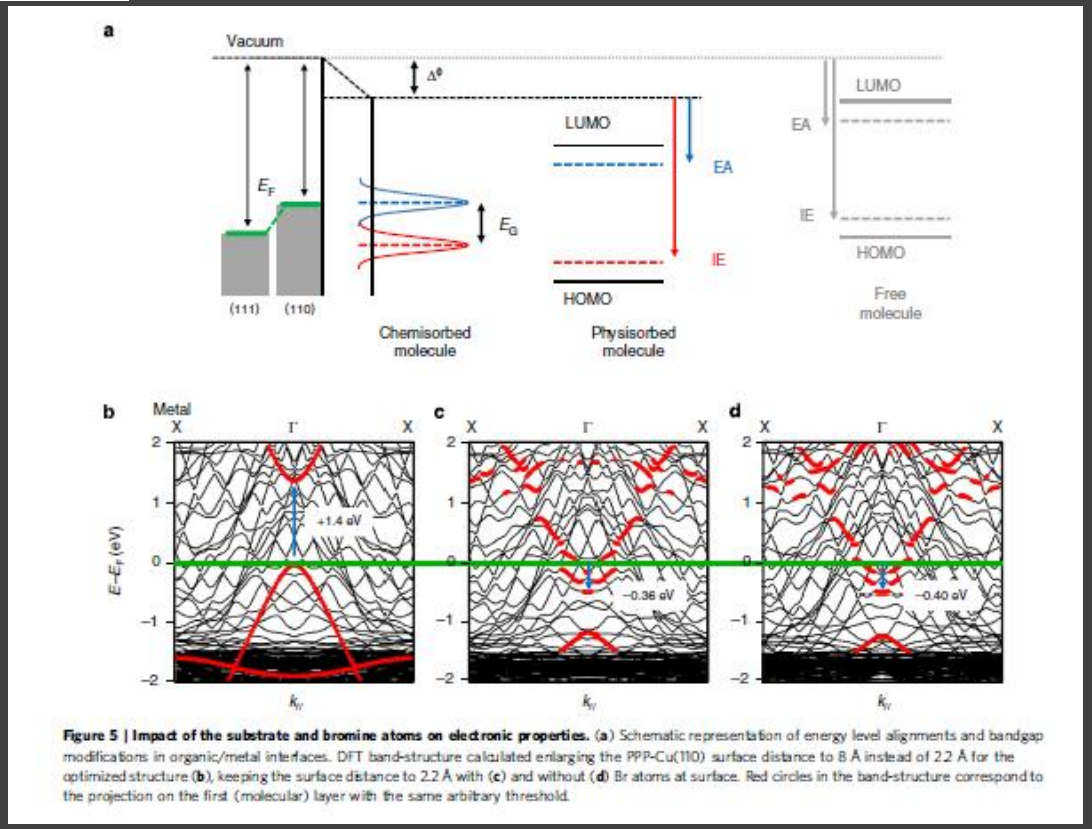
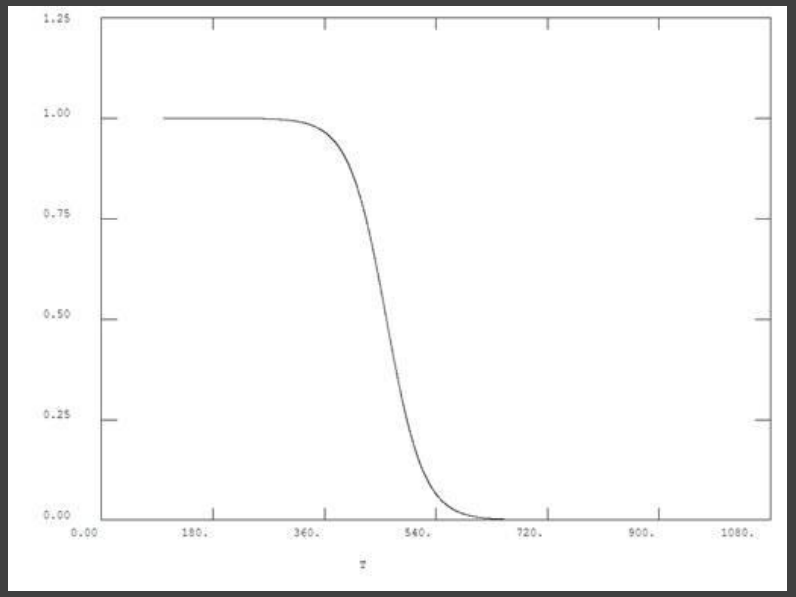
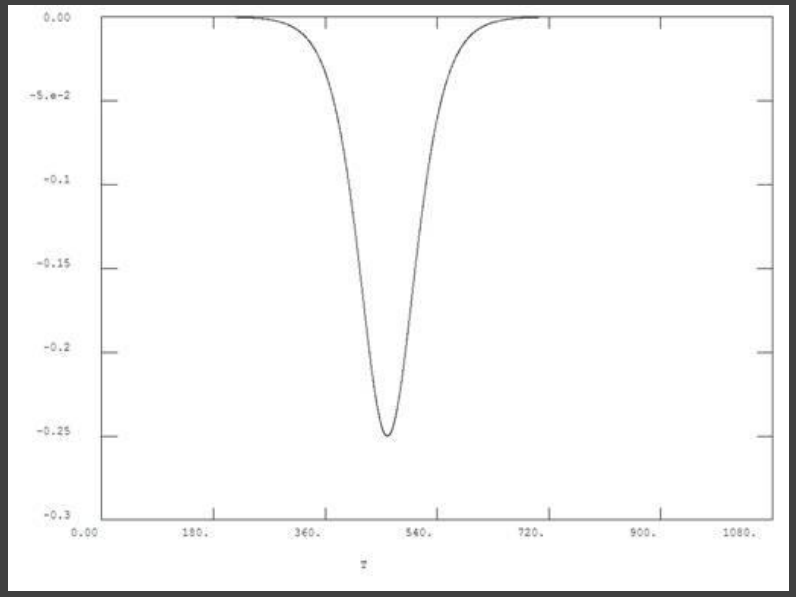


Figure 5 | Impact of the substrate and bromine atoms on electronic properties. (**a**) Schematic representation of energy level alignments and bandgap modifications in organic/metal interfaces. DFT band-structure calculated enlarging the PPP-Cu(110) surface distance to 8 Å instead of 2.2 Å for the optimized structure (**b**), keeping the surface distance to 2.2 Å with (**c**) and without (**d**) Br atoms at surface. Red circles in the band-structure correspond to the projection on the first (molecular) layer with the same arbitrary threshold.

Función de Fermi





Calor especifico