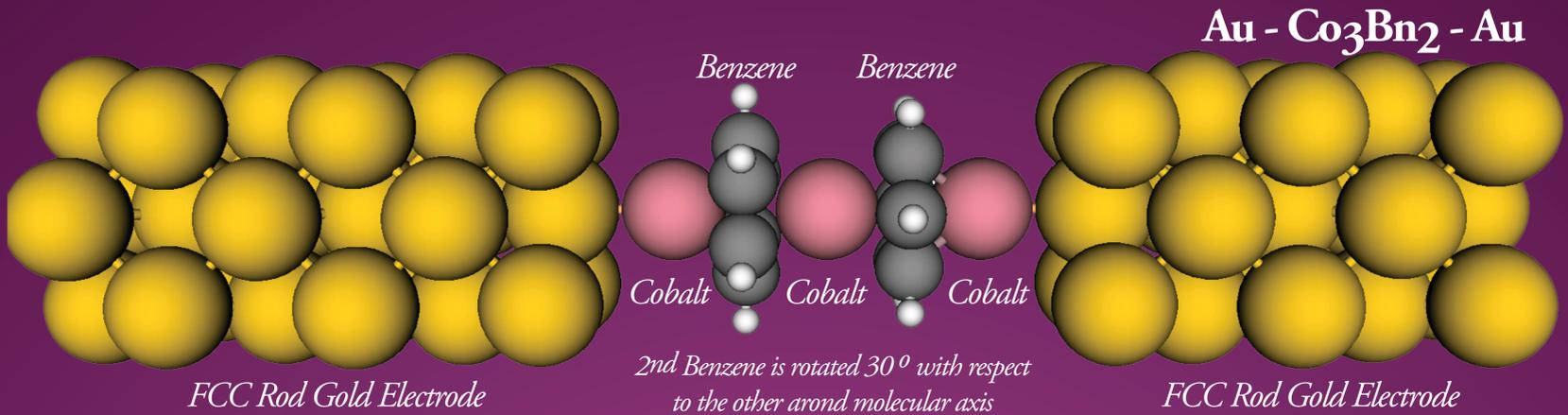


# ELECTRONIC AND TRANSPORT PROPERTIES OF COBALT - BENZENE NANOSTRUCTURES: A MOLECULAR SPIN VALVE

Ertuğrul Karademir, Department of Physics Bilkent University 06800 Ankara, Turkey



## SPINTRONICS

- Electronics with spin degree of freedom.
- Ideally, e.g. Spin Up = 1 Spin Down = 0.
- Spin polarized currents.

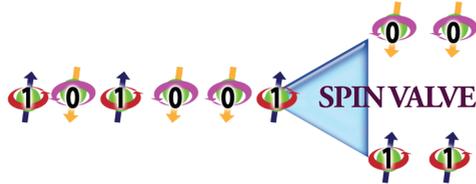


### USAGE

- Dense, fast, and non-volatile memory modules: MRAM
- Circa 2025 we will need more aggressive processing power, hence:
  - > Quantum Computers
- Already Intel processors employ few electrons per transistor.
- New applications will emerge as new materials are discovered.

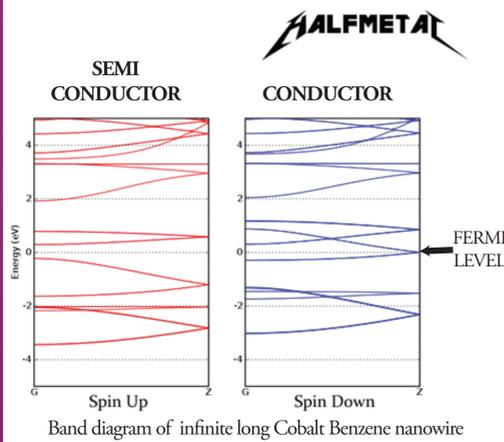


## SPIN VALVES

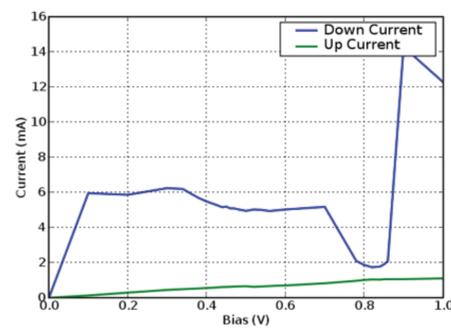
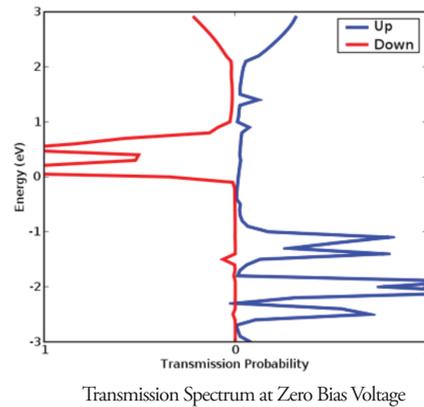


- Ideally separates electrons with different spins.
- Half metallic structures are good candidates.

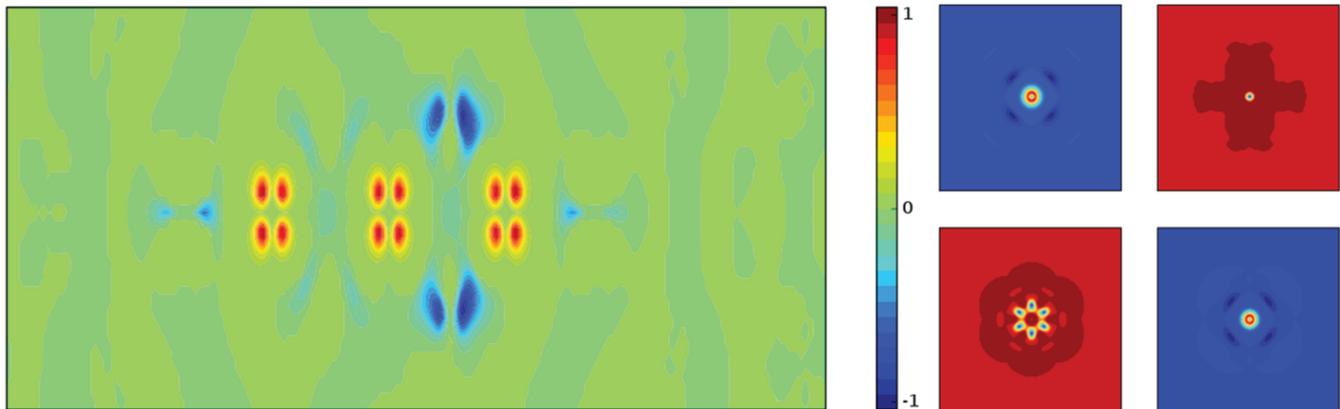
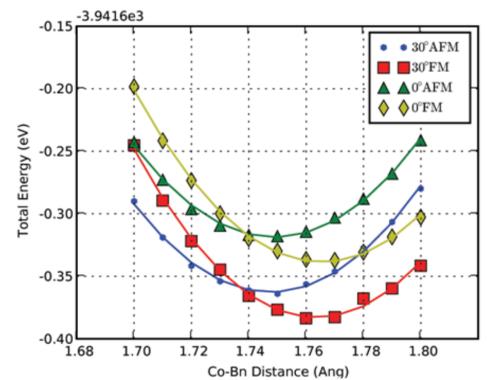
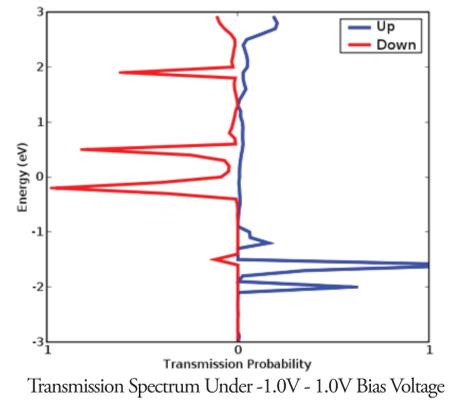
## HALF METALS



## COBALT BENZENE



## COBALT BENZENE



Electron spin density maps: These maps are generated by calculating electron density at a given coordinate. Density of electrons with spin down magnetic moment are subtracted from the density of spin up magnetic moment and normalized to the maximum and minimum of that result in whole space. Thus 1 means that at that point, electrons have the maximum SPIN UP moment, and -1 means that they have the maximum SPIN DOWN moment. With this method one can recognize the moment changes through the whole molecule. These maps are crosssections of A) molecular axis i.e. X=0 plane, B) 1)X-Y crosssection of first cobalt from the left, 2) second cobalt from left, 3) second benzene from the left, 4) third cobalt from left. This snapshot of electron distribution is taken under -0.36V, 0.36V bias voltage.

## METHODS

- At early stages of modelling of the device, we have optimized the formation of the unitcell by minimizing force calculations using Density Functional Theory.
- After optimization, we have probed the infinite long nanowire to determine the band diagram, which shows if the nanowire is a conductor, semi conductor, etc.
- After characterization of the infinite long nanowire, we have cleaved a finite part and connected this part with gold electrodes. Then we have optimized this new structure again.
- After the second optimization we have probed the device for Landauer ballistic transport properties.
  - > Transmission spectrums show the probability of electron transport at that energy level.
  - > Current under a bias voltage is calculated basically by integrating the part of the transmission spectrum marked by the range of bias voltage. -1V, 1V bias means that the range of the integral is from 1eV below the Fermi level to 1eV above.

