Rosa Di Felice (INFM National Center for nanostructures and BioSystem at Surfaces, Modena) Theoretical investigation of metal-coating DNA-based helices
e-mail: rosa@unimore.it

Why exploring charge carriers in metal-containing biomolecules. Focus on DNA bases complexes (quadruplex G4-DNA), ground state single particle electronic properties. Is DNA a viable electrical material? Experiments show DNA charge mobility is poor. For molecules attached to substrates. Use stiffer molecules or softer surfaces. Can also improve intrinsic conductivity through metal insertion. Metal-DNA interaction: different contexts - more interested in metals inside the helix. Guanine based DNA or metalized DNA. Use Density functional theory-GGA, ultrasoft psuedopotential, plane waves, etc. quadruple helices (G4-wires). X-ray structure is available: it is characterized by square and translation symmetries, K^+ are interplanar. The backbone is neglected in the simulation. Double ring of H-bonds, electronegative inner core, monovalent cations make G-wires thermodynamically stable, no in plane delocalized orbital bonding. K(I) G4 Electronic Structure: flat bands, no dispersion along wires axis, manifolds, effective semiconductor. Channels for charge motion through the bases, poor potassium-guanine coupling. Redox-active metals in G4-wires - Cu(I)G4: Cu integrates into plane. Cu(II) is more interesting, spin down state can accept electrons. Have played with different ion incorporation, but no successful experimental results. Metal incorporated wires - substitution of GC with hydroxypyridone. Spin density is a linear combination of spin up and spin down, strong coupling between metal and base. Electronic structure, 5 band manifolds originate peaks in the DOS, filled π-like HOMO, partially filled sigma orbitals, ferromagnetic alignment.