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Unveiling the electronic properties of Metallo-DNA nanowires

Arpan De

Department of Electrical and Computer Engineering, University of Washington, Seattle, USA
Experimental Collaborators: James W Canary Group, New York University, USA

PhD Supervisor: Prof. M. P. Anantram

Introduction

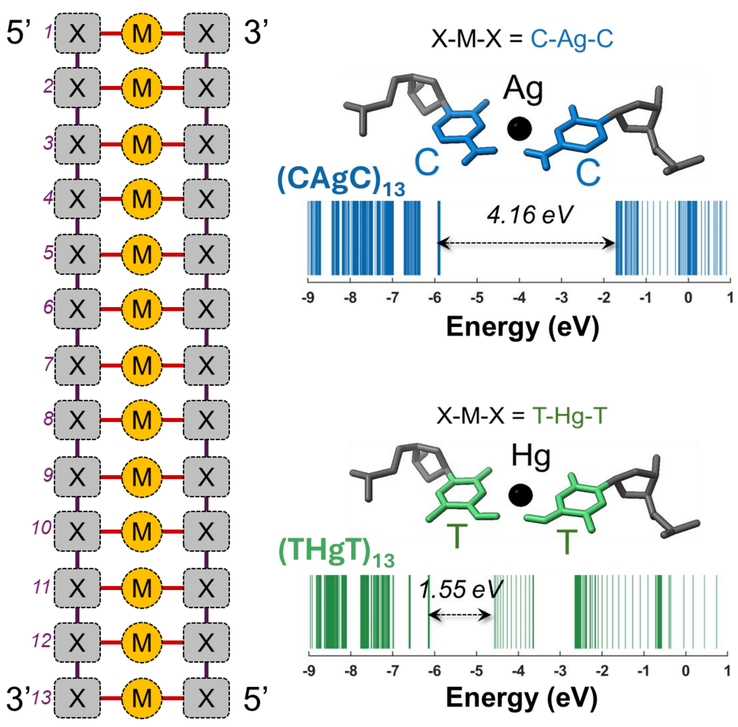
- Nucleic acid modification *via* metal coordination is a promising approach for expanding applicability of DNA nanoelectronics.
- Long metallo-DNA nanowires with stacked "metallobases" has been experimentally demonstrated (J Kondo *et al.*, S Copp *et al.*).

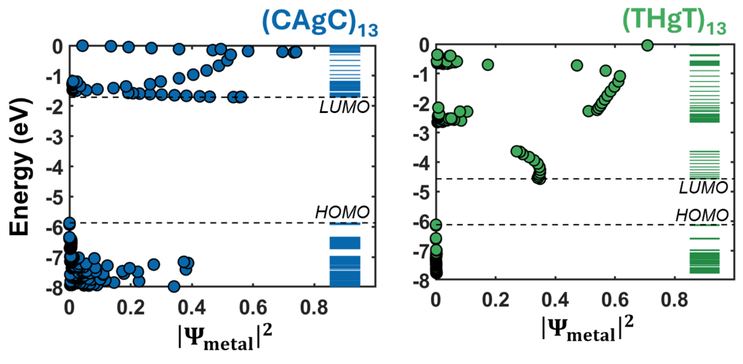
Methodology

- Density Functional Theory (DFT) with B3LYP/6-31g(d,p) and LANL2DZ.
- Green's function-based Transport modeling:

$$[E - H - \Sigma_L - \Sigma_R]G^r = I$$
$$T(E) = trace\left(\Gamma_L G^r \Gamma_R (G^r)^\dagger\right)$$
$$[\Gamma_{L,R} = -2Im\left(\Sigma_{L,R}\right)]$$

Energy Eigenvalues



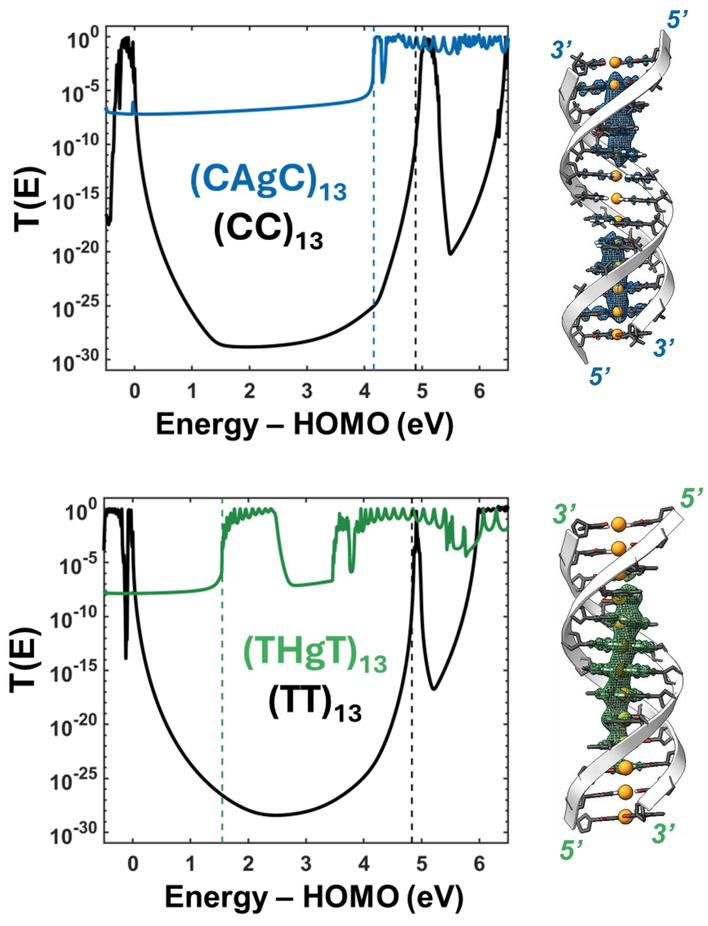


- Two 13-bp long metallo-DNA nanowires considered: $(CAgC)_{13}$ and $(THgT)_{13}$.
- *Ag* modifies energy levels near the LUMO of non-metalated DNA nanowire, while *Hg* adds states inside the bandgap.
- LUMO Contribution of metal in $(CAgC)_{13}$ is 0.56 while that in $(THgT)_{13}$ is 0.37.

Key Points

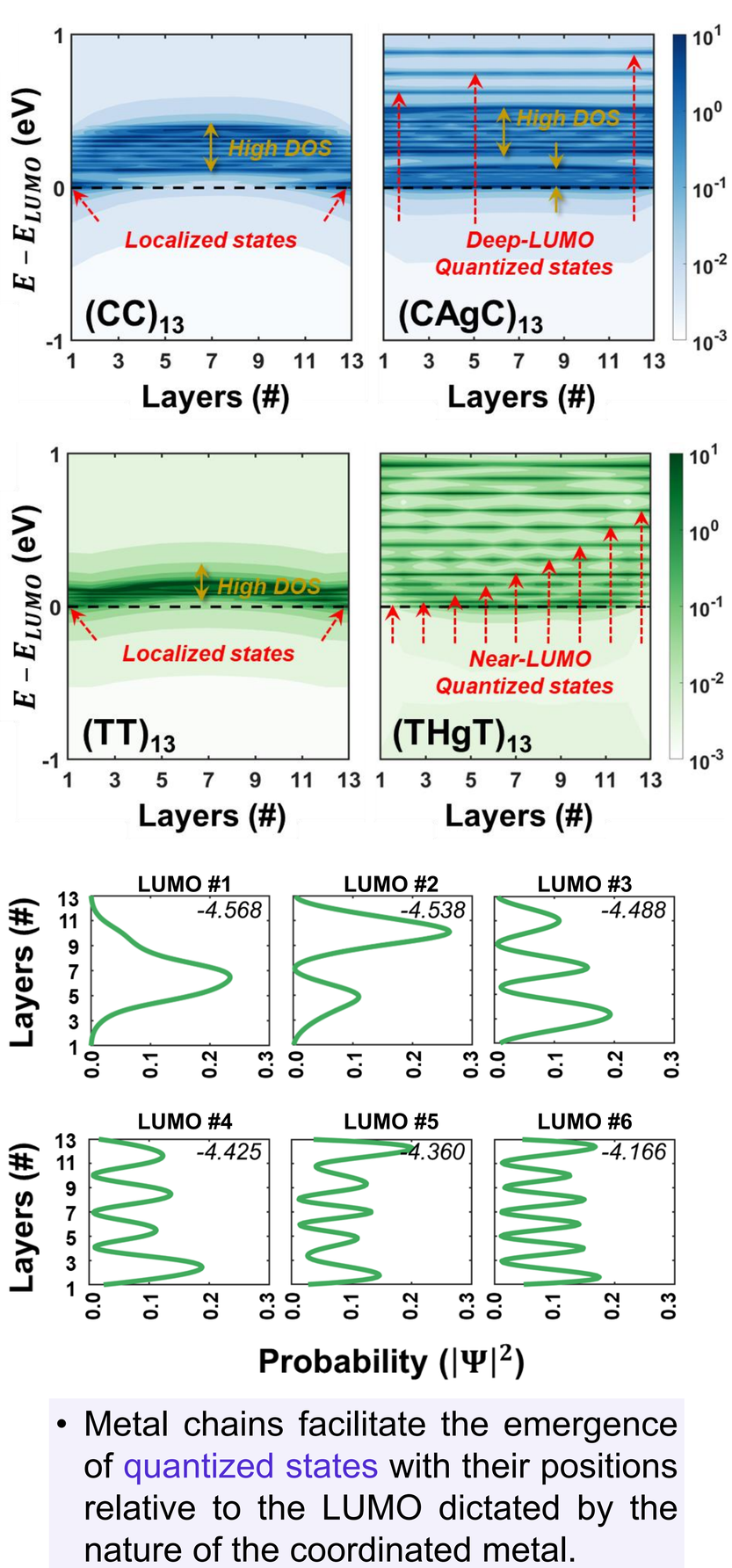
- Significant HOMO-LUMO gap reduction.
- Broadening of LUMO band.
- Enhanced coupling energies between LUMOs.
- $(THgT)_{13}$ exhibits particle-in-a-box (PiB) behavior.
- Electronic applications: DNA-conductor and 1D-topological insulators*.
- Metallo-DNA nanowire governed by relativistic heavy-metal physics** and quantum confinement, generating robust, tunable electronic states with readily verifiable spectroscopic and transport signatures.

Transport Properties



- LUMO transmissions in $(CAgC)_{13}$ and $(THgT)_{13}$ are significantly higher than that of their non-metalated counterparts.
- LUMO bandwidth (up to 1 eV) is larger due to enhanced coupling between metalated base pairs.
- Partial density of states on 13 metals is large at LUMO states.
- We demonstrate that a periodic metal-modified DNA, which contains only one metal atom per base pair, gives rise to metal-centered electronic bands rather than localized impurity-like states.

Metal-modulated DOS



- Metal chains facilitate the emergence of quantized states with their positions relative to the LUMO dictated by the nature of the coordinated metal.
- High DOS regions form at energy levels with minimal metal contribution and arise primarily from the conjugation between the DNA and the metal chain or, in some case, due to the DNA alone.

(Group Website)

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