ARPAN DE, PARITOSH SINGH

Abstract

DNA is a promising candidate for nanoelectronics applications due to its customizable base sequence, low-cost replication, and self-assembly capabilities. While native DNA is a poor conductor and sensitive to environmental conditions, its conductivity and stability significantly improve when intercalated with metals, making it more robust and suitable for electronic integration.

Theory and Method

Density Functional Theory:

Used to calculate ground state energy (E) and Hamiltonian (H_0)

Transport

$T_{mn} = \Gamma_m G^r \Gamma_n (G^r)^\dagger$, where

$G^r = [EI - (H_0 + \Sigma_L + \Sigma_R + \Sigma_B)]^{-1}$ and $\Gamma_i(E) = -2Im\,(\Sigma_i)$

Here G^r is the retarded Green's function and $\Sigma_{L/R}, \Sigma_B$ are the self energy of left/right contacts and Buttiker probes respectively.

DNA as a device

- Electrical devices are an engineered arrangement of energy levels.
- DNA offers stability, adjustable energy levels, self-organization, and programmability.

Challenges

- Binding energies between bases ~ 100-130 meV in their native form
- Low electron hopping integral (10-100 meV)

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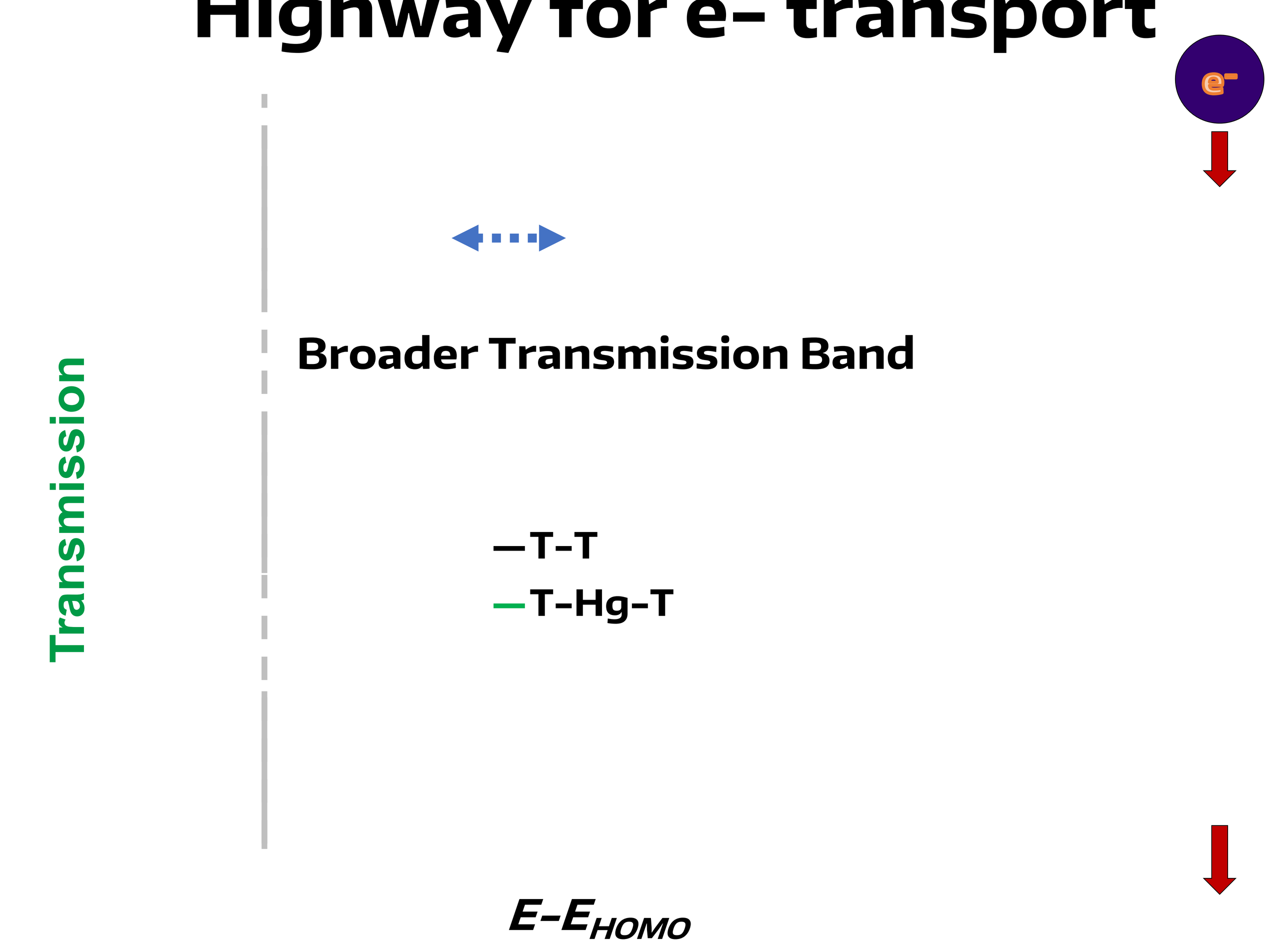
Metal Intercalated Base Pairs

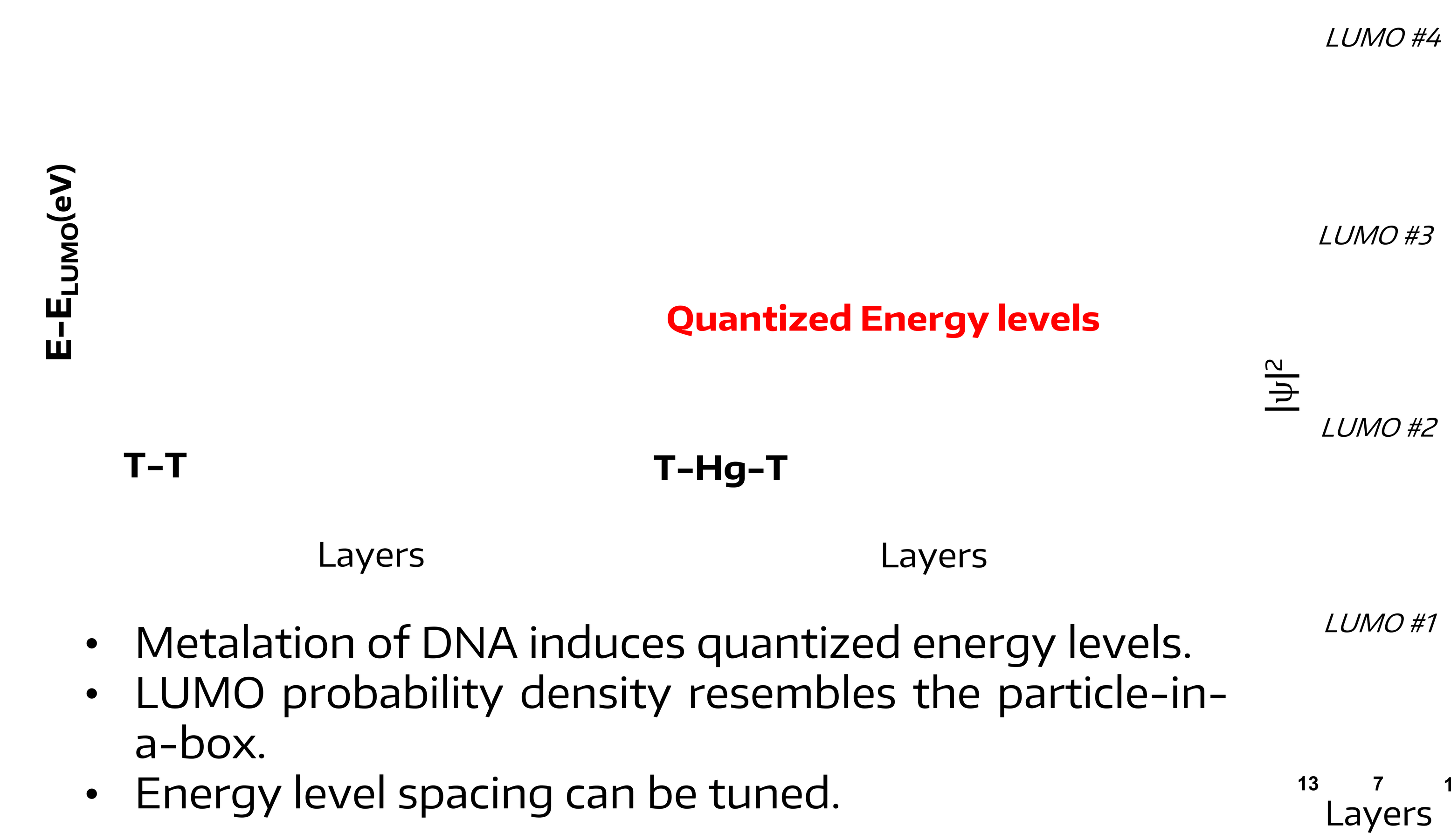
- Intercalating metal atoms enhance binding energy between bases
- It lowers the DNA band gap and increases electron hopping energy

Highway for e- transport



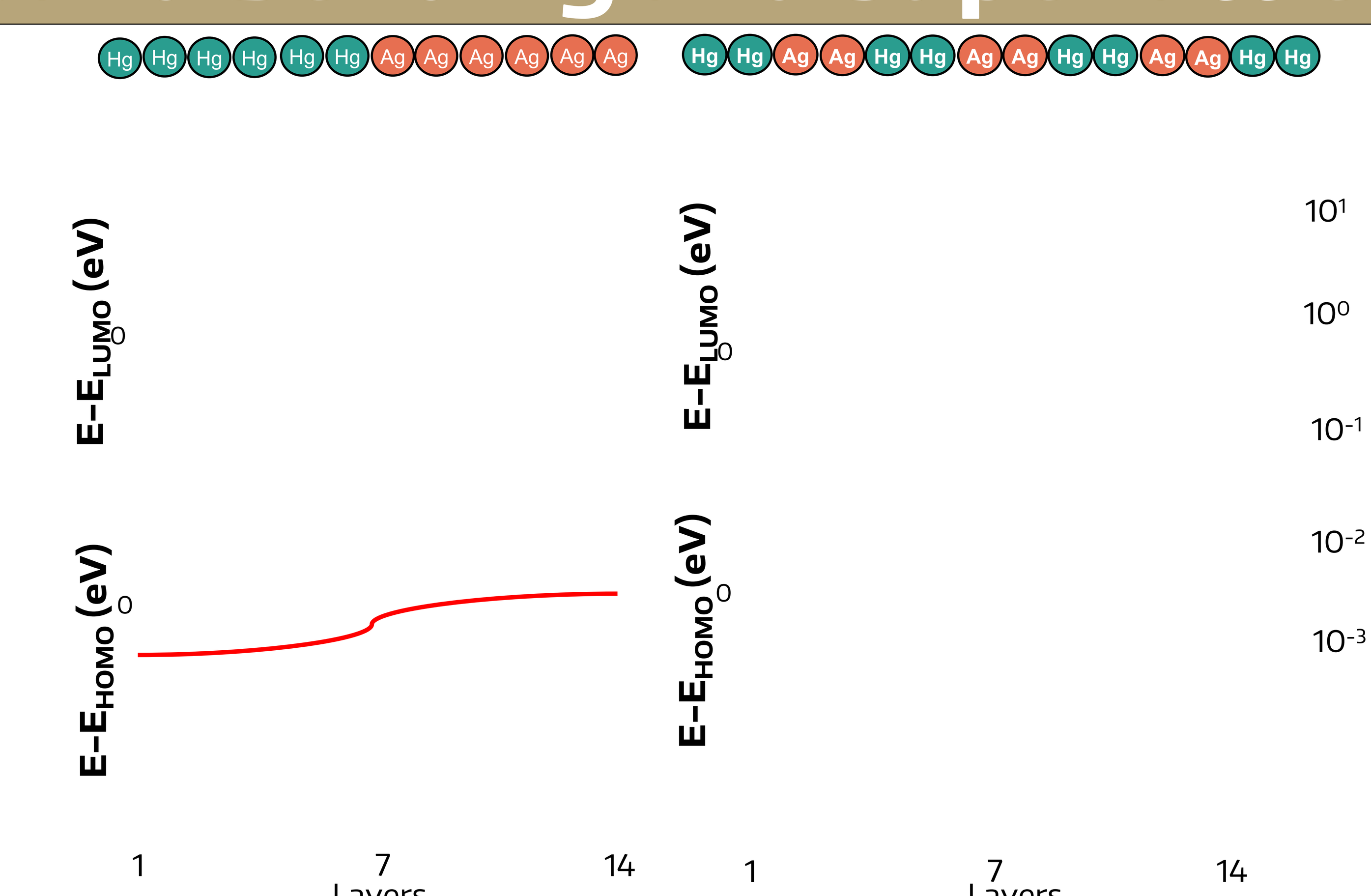
- Metal atoms introduce energy levels in the band gap of DNA
- It increases the conductivity across a wide band of energies as depicted by the broader transmission band.

Energy Quantization



- Metalation of DNA induces quantized energy levels.
- LUMO probability density resembles the particle-in-a-box.
- Energy level spacing can be tuned.

Band Bending and Superlattices



DOS representing band bending (left) and superlattice (right)

Conclusion

- Metal intercalation enhances the conductivity and stability of DNA nanowires.
- *Strong* transmission path is possible at the LUMO of T-Hg-T
- Electronic properties can be tailored: superlattices and band bending.
- It presents an engineered nanomaterial to probe molecular scale band engineering

References

- De, Arpan, et al. /doi.org/10.26434/chemrxiv-2025-nkbgv.
- Vecchioni, Simon et al., doi:10.1002/adma.202210938
- J. Kondo *et al.*, doi: https://doi.org/10.1038/nchem.2808.