DNA OR AN ELECTRONIC COMPONENT? THEY ARE CLOSER THAN YOU THINK

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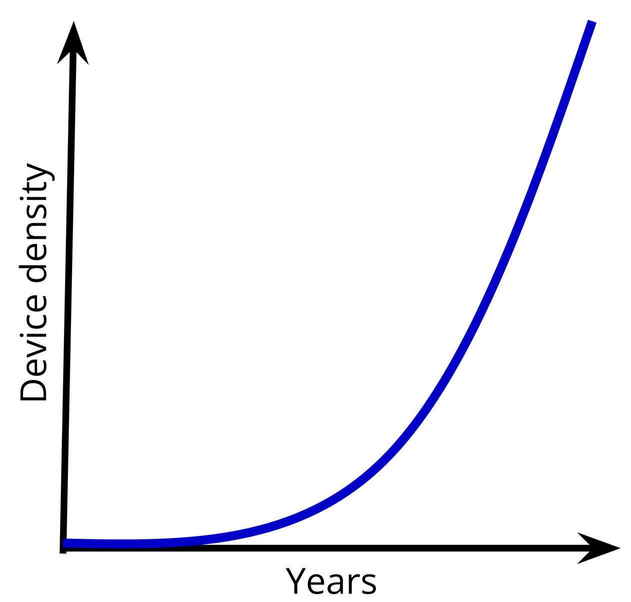
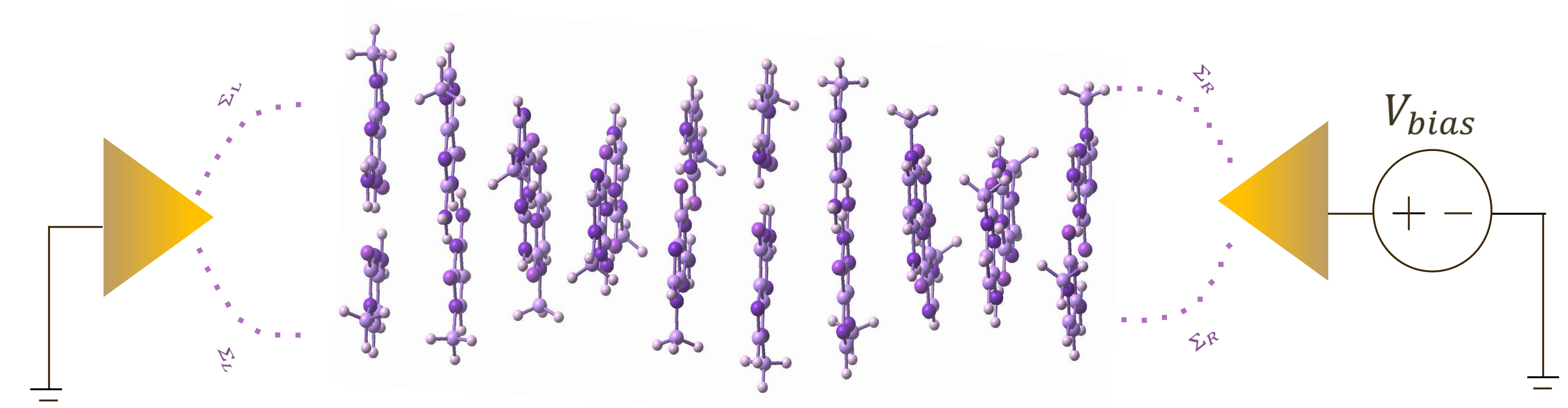
MOTIVATION



- Devices getting smaller
- DNA self-assembly has **atomic-level precision**
- See how to **engineer conductance** with different sequences
- Study electrical **properties**
- No inelastic scattering in previous studies

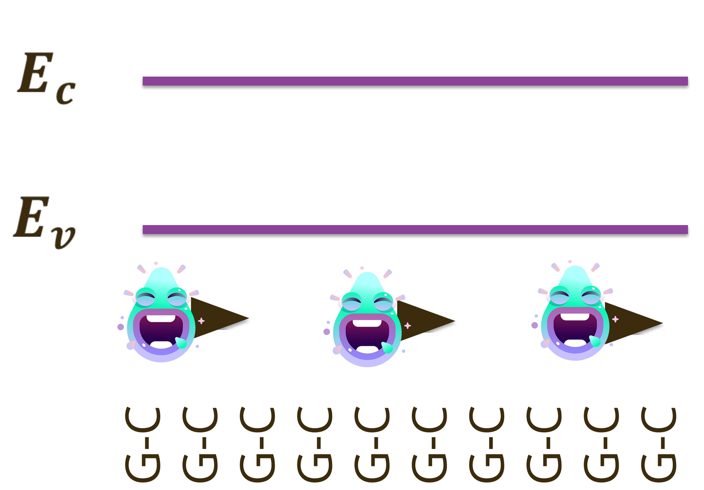
SETUP



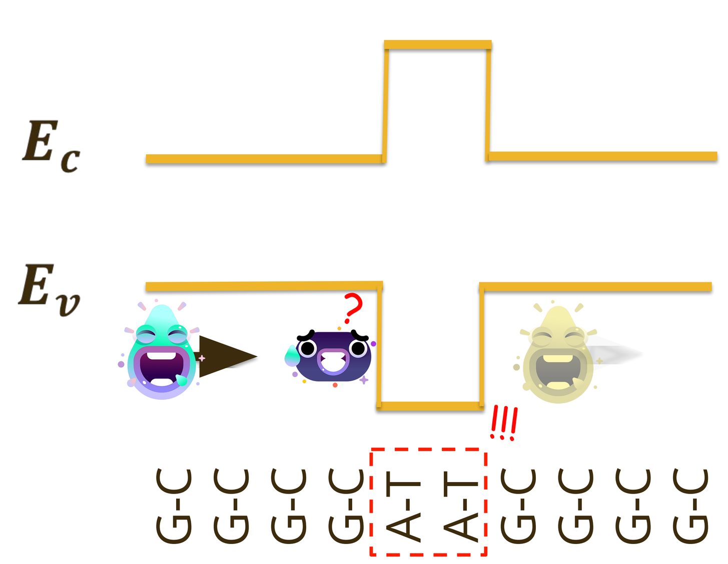
Poly(G) DNA strand (backbone replaced with $-CH_3$) is probed at the left and right base pairs

Environmental decoherence is modeled with dephasing probes

MODEL APPROXIMATION

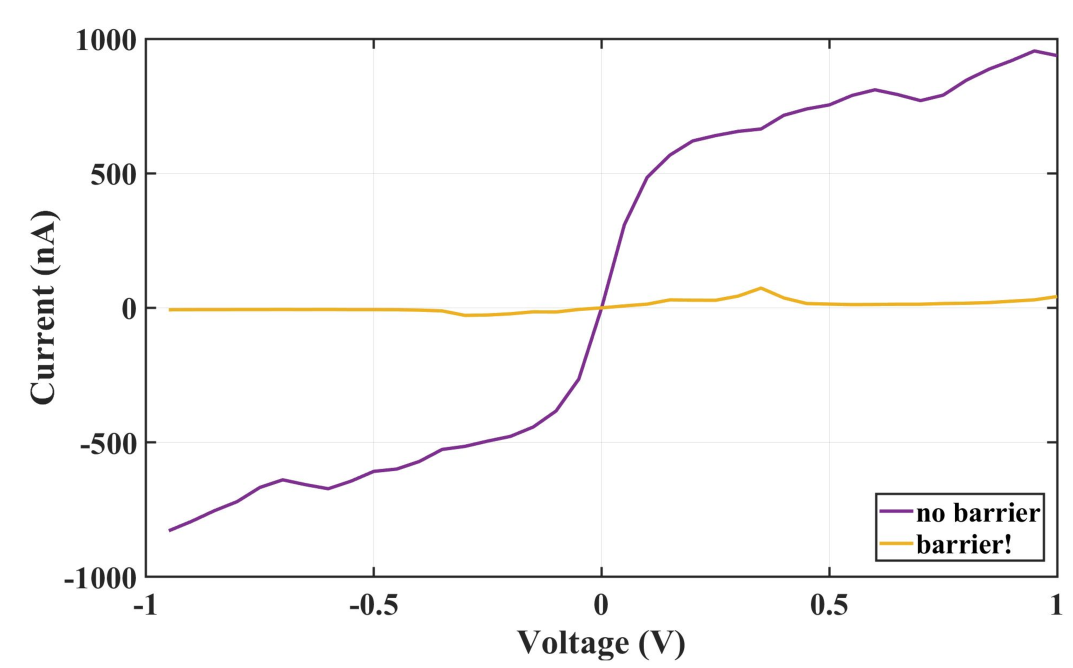


- G-C base pair has a low ionization energy, **conductance is observed to be high** compared to other nucleic acids

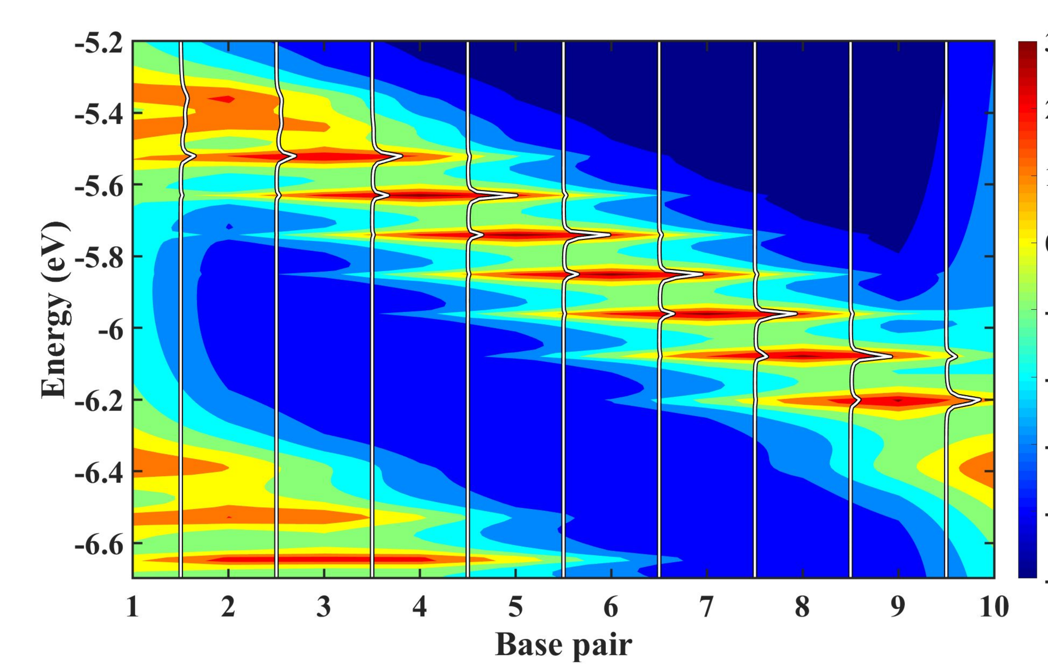


- A-T base pair acts as a **hole barrier**

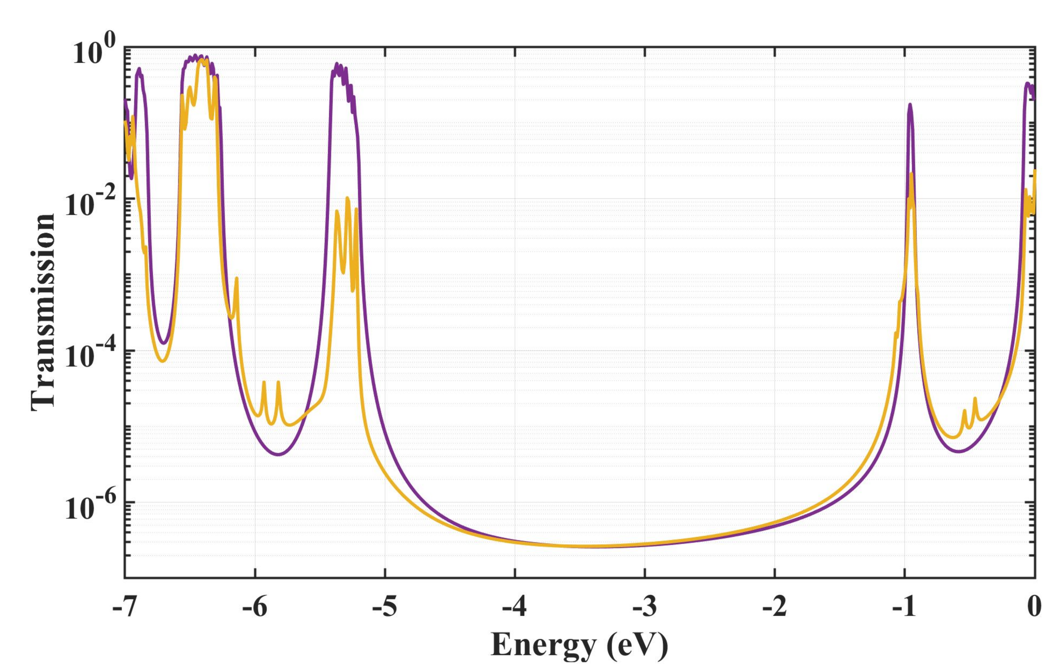
RESULTS



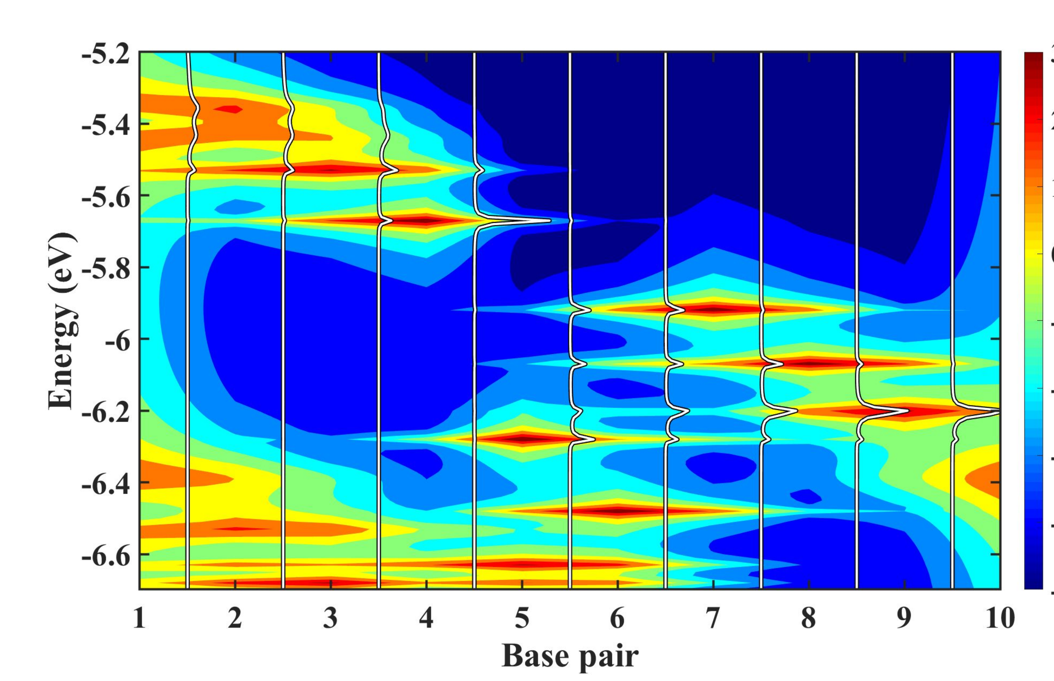
- Current-voltage curve shows current shuts off with sequence modification



- Local density of states (LDOS) allows for a path for current. Current through DNA cross-sections is shown (no barrier)



- Transmission with and without a barrier shows drastic decline at resonant energies



- LDOS and current (amplified by 30 for visuals) with the hole barrier

KEY FINDINGS

1. **Monotonic increase in current** without a barrier – purely coherent models fail to reproduce physical I-V behavior
2. Inclusion of a hole barrier suppresses hole-channel transmission by ~100x, demonstrating **sequence-controlled conductance switching**
3. Spatial LDOS maps reveal a well-defined intra-molecular **conduction pathway** — current cascades through stacked guanine bases via **sequential hopping**
4. Base-sequence programmability enables bottom-up design of molecular switches — a stepping stone toward **DNA-based nanoelectronic components**

METHODS

- Transmission
$$\begin{cases} [E-(H+\Sigma_L+\Sigma_R+\Sigma_B)]G^r = I \\ T(E) = Tr[\Gamma_L(E)G^r(E)\Gamma_R(E)G^a(E)] \end{cases}$$
- Current $I_L = \frac{2q}{h}\sum_{j\in probe}\int T_{L,j}(E) * \left[f_L(E) - f_j(E)\right] dE$
- Chemical potential of probes is determined by:

$$\begin{bmatrix}\mu_1\\ \mu_2\\ \vdots\\ \mu_N\end{bmatrix}_{itr+1} = \begin{bmatrix}\mu_1\\ \mu_2\\ \vdots\\ \mu_N\end{bmatrix}_{itr} - \alpha \begin{bmatrix}\frac{\partial I_1}{\partial \mu_1} & \frac{\partial I_1}{\partial \mu_2} & \cdots & \frac{\partial I_1}{\partial \mu_N}\\ \frac{\partial I_2}{\partial \mu_1} & \frac{\partial I_2}{\partial \mu_2} & \cdots & \frac{\partial I_2}{\partial \mu_N}\\ \vdots & \vdots & \ddots & \vdots\\ \frac{\partial I_N}{\partial \mu_1} & \frac{\partial I_N}{\partial \mu_2} & \cdots & \frac{\partial I_N}{\partial \mu_N}\end{bmatrix}^{-1} * \begin{bmatrix}I_1\\ I_2\\ \vdots\\ I_N\end{bmatrix}_{itr}$$

FUTURE WORK

- Characterize barrier-length dependence of tunneling regime — transition from direct to **Fowler-Nordheim tunneling**
- Model effects of a **phosphate backbone** with charged termination groups
- Observe the nucleotide behavior when an **additional electron** is added to the system

(Group Website)

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