

Title: Transport in molecular scale

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URL: <http://pirsa.org/13120021>

Abstract: <span>Recently there has been a large growth of research effort for nanoelectronic devices. Investigations of quantumly coherent nano-meter scale systems whose fabrication has been made possible by recent advances in experimental and sample preparation techniques have revealed that transport properties could be non-Ohmic and  $G$  could be quantized. Understanding electron conduction in such devices is an extremely active research topic. Our theoretical goal is to predict quantum transport properties of molecular nanodevices including their I-V characteristics from first principle theoretical method.</span>

# Transport in Molecular Scale Systems

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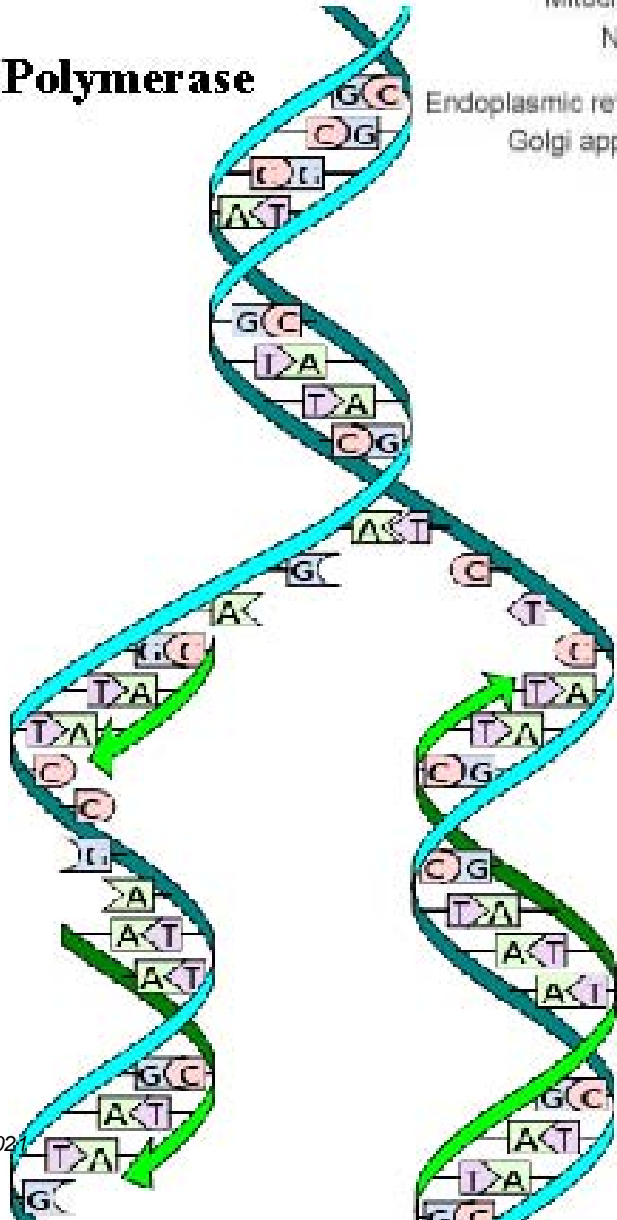
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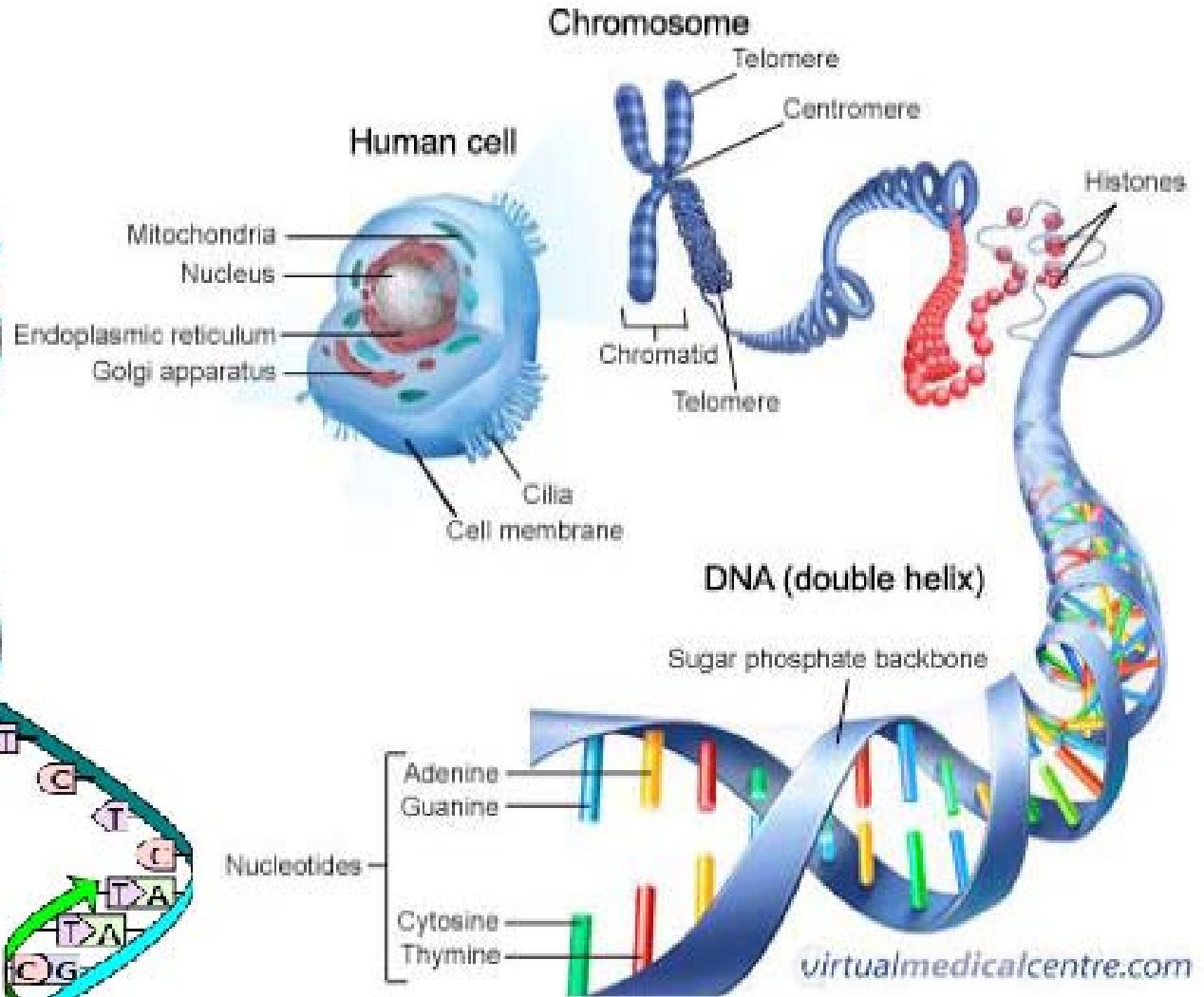
# DNA Sequencing:

## DNA Replication

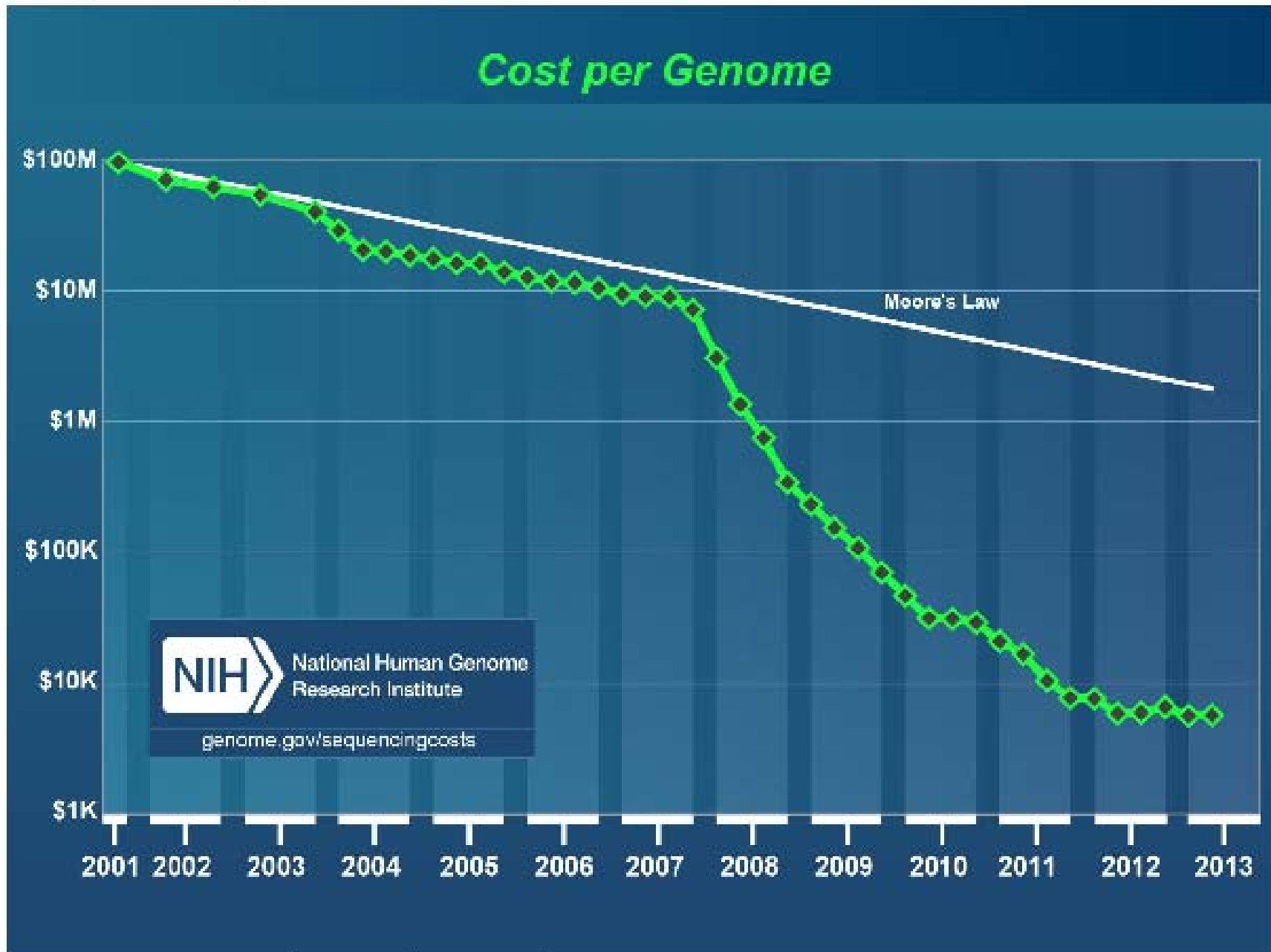
## DNA Polymerase



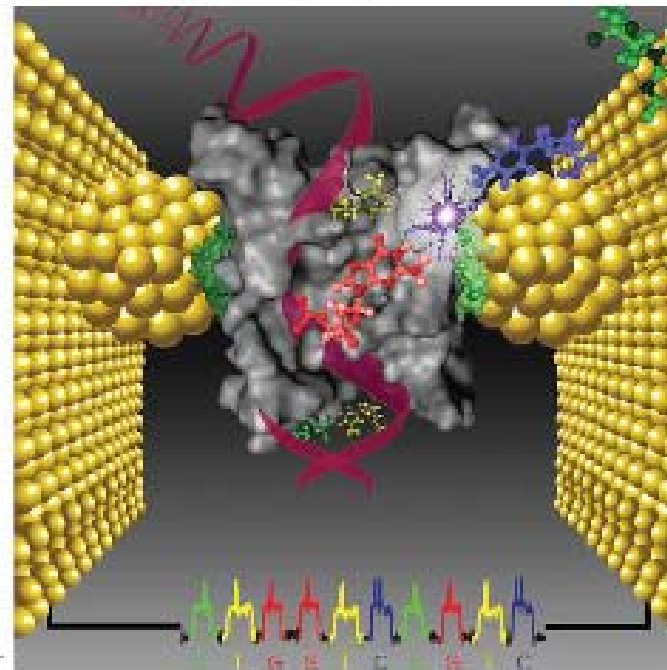
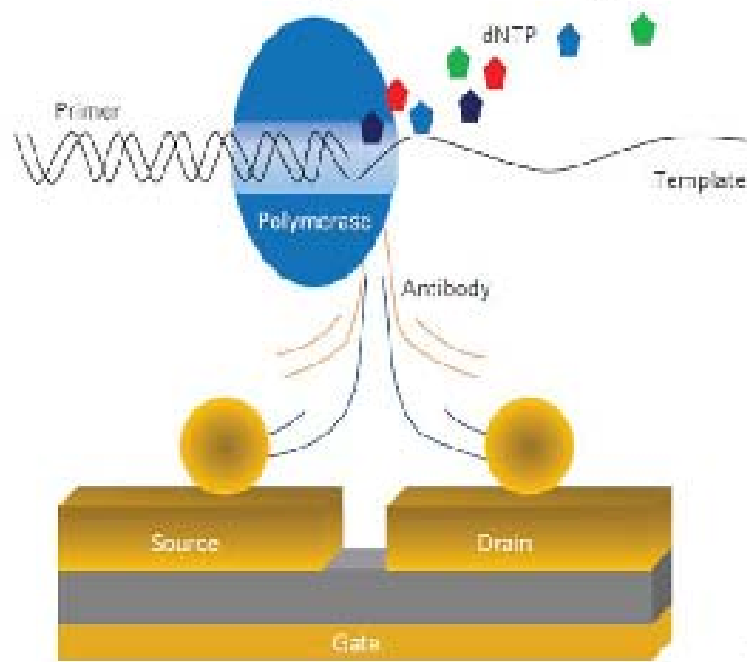
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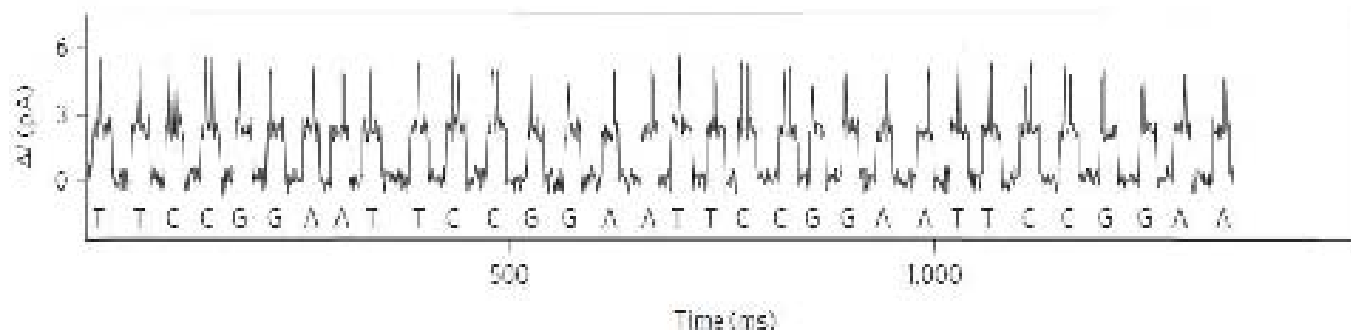
# DNA Sequencing:



# Experimental Progress The protein transistor-DNA polymerase device



Schematic representation of the single-molecule sequencing platform.



# Theoretical Formalism

Kohn-Sham equations for an open system

Kohn-Sham potential is effectively screened

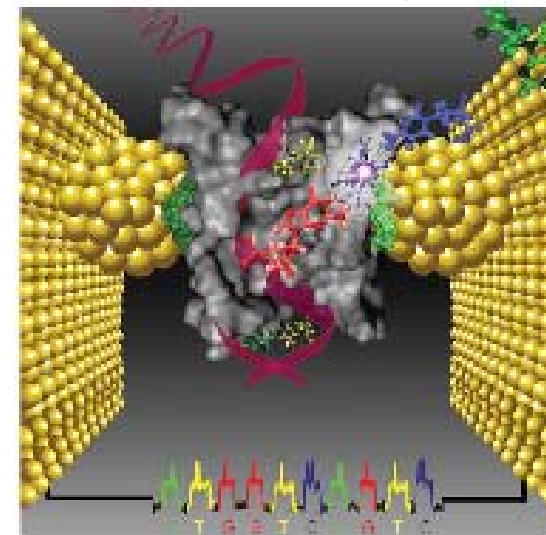
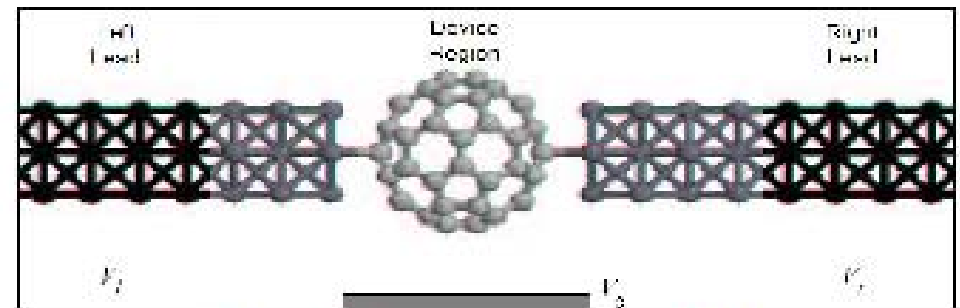
Infinite problem

Finite scattering or device region

Effective potential

Basis set to construct the Hamiltonian

Density matrix from non-equilibrium Green's function



$$\hat{\rho} = -\frac{i}{2\pi} \int dE G^<(E),$$

$$G^< = G^R \Sigma^< [f_l^{k_l^n}, f_r^{k_r^n}] G^A$$

$$\Sigma^< [f_l^{k_l^n}, f_r^{k_r^n}] = -2i \text{Im}(f_l^{k_l^n} \Sigma_{l,i}^l + f_r^{k_r^n} \Sigma_{r,r}^r).$$