Torsional Vibration Dependence on Transport Properties of DNA Molecules

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Regional School on Physics at the Nanoscale, Dec. 2009, Hanoi, Vietnam


Traffic
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Terrain
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Dumai
Johor
Singapore
Natal
Sosa
Sungai Apit
Hibala
Batahan
Tembilahan
Sumpur Kudus
Kumpeh
Muara Padang
Banyuasin II
Bengkulu Utara
Palembang
Tulung Selapan
Cengal
Bengkulu
Pakuan Ratu
Lemong
Bandar Lampung
Jakarta
Semarang
Surabaya
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Malang
Tegaldimo
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Christmas Island
Bunguran Timur
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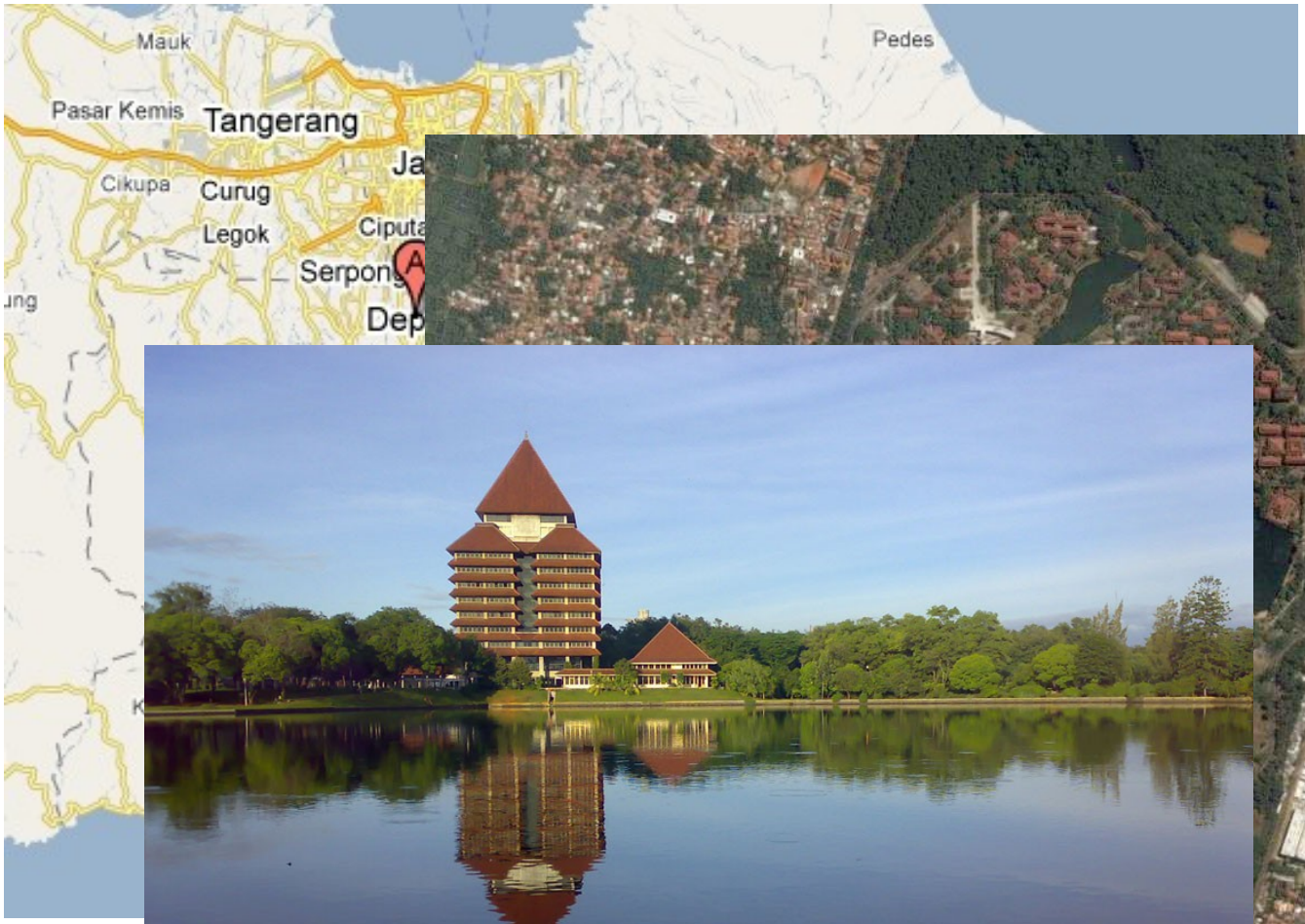
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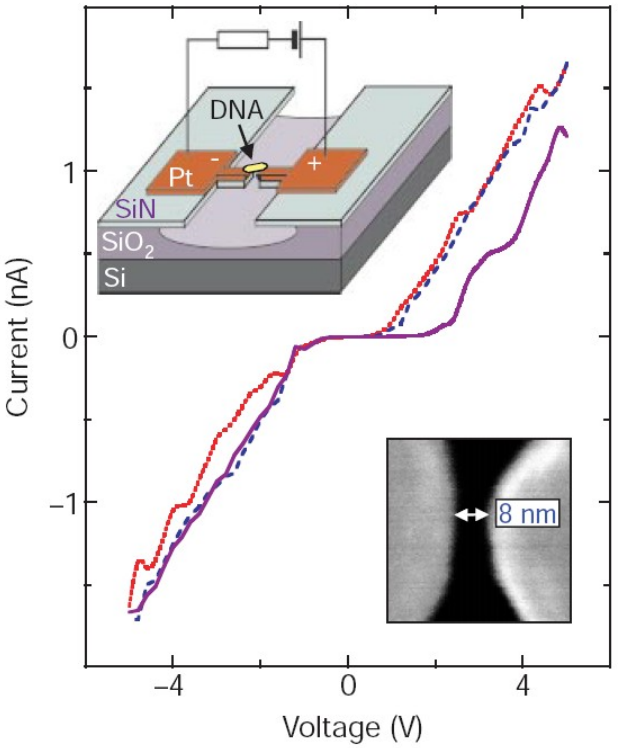
Outline

- **Motivation**
- **Torsional vibration dependence on transport properties of DNA molecules.**
- **Phonon effects on charge transport through a DNA base pair.**

Motivation

- **Molecular electronics**
- **Charge transfer in biology**
- **DNA can range from insulator to ohmic; Endres *et al.*,** Rev. Mod. Phys. **76**, 195 (‘04)
- **Conductivity depends on temperature; Yoo *et al.*,** Phys. Rev. Lett.**87,** 198102 (’01)**, Tran et al.**, Phys. Rev. Lett. **85**,1564 (’00)
- **Studying the effect of phonons**



30 bps poly(G)-poly(C)
large band-gap semiconductor

(Porath *et al.*, Nature **403**, 635, (2000)**)**

Torsional vibration dependence on transport properties of DNA molecules.

Daniel Kurnia, Efta Yudiarsah, and Rosari Saleh
Universitas Indonesia

The effect of temperature

Ordered *sequence*→ Poly(dG)-poly(dC)

Disordered *sequence*→ Modified Poly(dG)-poly(dC): 50 GC base pairs replaced with 50 AT, TA, or CG base pairs

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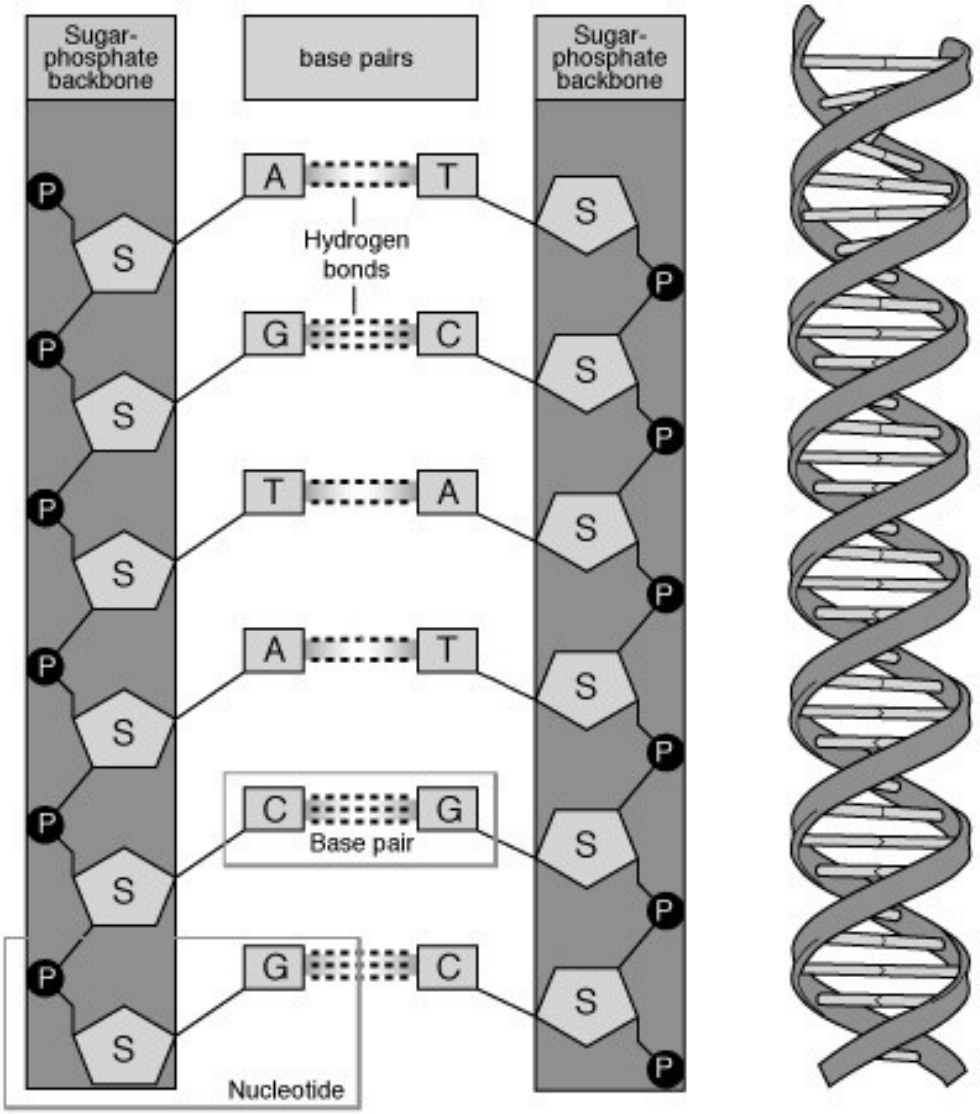
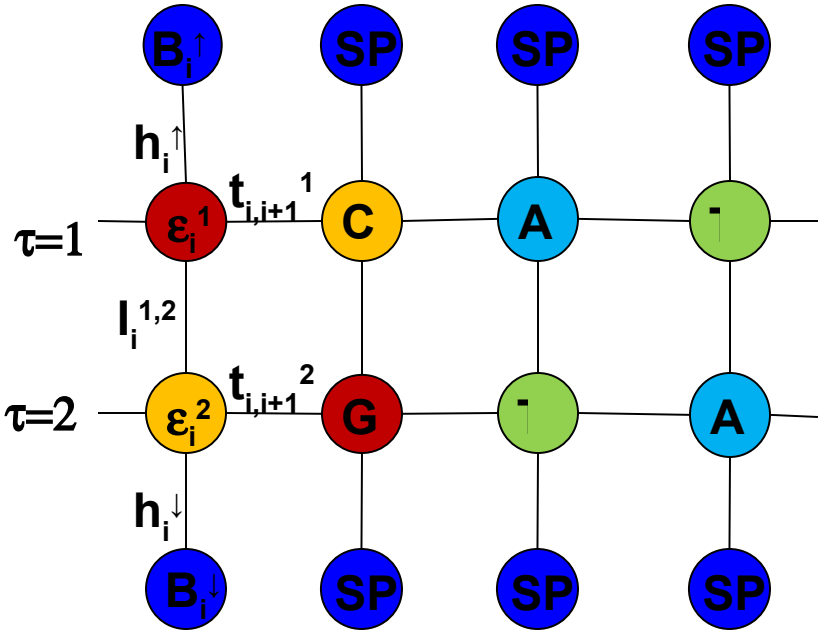
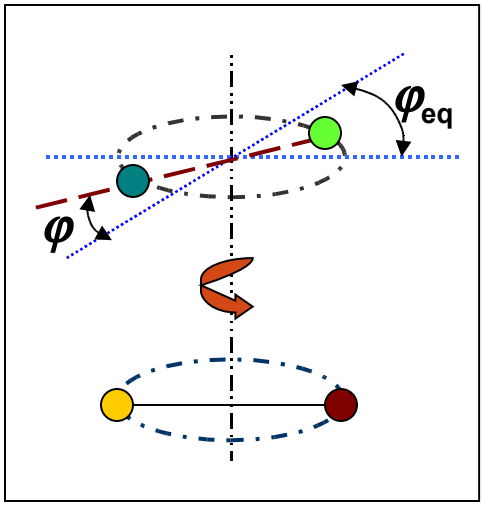
DNA Structure



2-Channel Model



100 base pairs long DNA sequence



Relative angle between two adjacent base pairs.

Angle follows a Gaussian distribution with zero average and standard deviation $\sqrt{\frac{T}{f}}$ → temperature

→ ~ ω^2

Hamiltonian

$$H = \sum_{i=1}^{L} \left[\sum_{\tau=1}^{2} \left\{ \left(\varepsilon_i^{\tau} + \phi_i^{\tau} \right) \left| i,\tau \right\rangle \left\langle i,\tau \right| + t_{i,i+1}^{\tau} \cos\Delta_{i,i+1} \left(\left| i,\tau \right\rangle \left\langle i+1,\tau \right| + \text{h.c.} \right) \right\} \right.$$

$$+ \sum_{q=\downarrow}^{\uparrow} B_i^q \left| i,q \right\rangle \left\langle i,q \right| + \sum_{\{\tau,q\}=\{1,\downarrow\}}^{\{2,\uparrow\}} h_i^q \left(\left| i,\tau \right\rangle \left\langle i,q \right| + \text{h.c.} \right)$$

$$\left. + I_i \left(\left| i,1 \right\rangle \left\langle i,2 \right| + \text{h.c.} \right) \right]$$

$$\phi_i^{\tau} = c_{i-1,i}^{\tau} \left(\cos\Delta_{i-1,i} - \cos\varphi_{eq} \right) + c_{i,i+1}^{\tau} \left(\cos\Delta_{i,i+1} - \cos\varphi_{eq} \right)$$

$$\Delta_{i,i+1} = \varphi_{eq} - \left(\varphi_i - \varphi_{i+1} \right)$$

$$\Delta_{i-1,i} = \varphi_{eq} - \left(\varphi_{i-1} - \varphi_i \right)$$

ε_G=7.84 eV, ε_A=8.22 eV, ε_C=8.85 eV,
ε_T=9.06 eV, and ε_B=9.36 eV

Transfer Matrix

Forward

$$\begin{pmatrix} \psi_{i+1} \\ \psi_{i} \end{pmatrix} = T_i \begin{pmatrix} \psi_{i} \\ \psi_{i-1} \end{pmatrix}$$

Backward

$$\begin{pmatrix} \psi_{i-1} \\ \psi_{i} \end{pmatrix} = T_i^b \begin{pmatrix} \psi_{i} \\ \psi_{i+1} \end{pmatrix}$$

$$T = T_1^b T_2^b \cdots T_{L-1}^b T_L^b T_L T_{L-1} \cdots T_2 T_1$$

Ndawana *et al.*, Europhys. Lett.**68**, 678 ('04)

Start with orthonormal matrix. Multiply with transfer matrix. Orthonormalized every n steps. Keeping the coefficients (α). Repeat *K* times

Lyapunove exponent

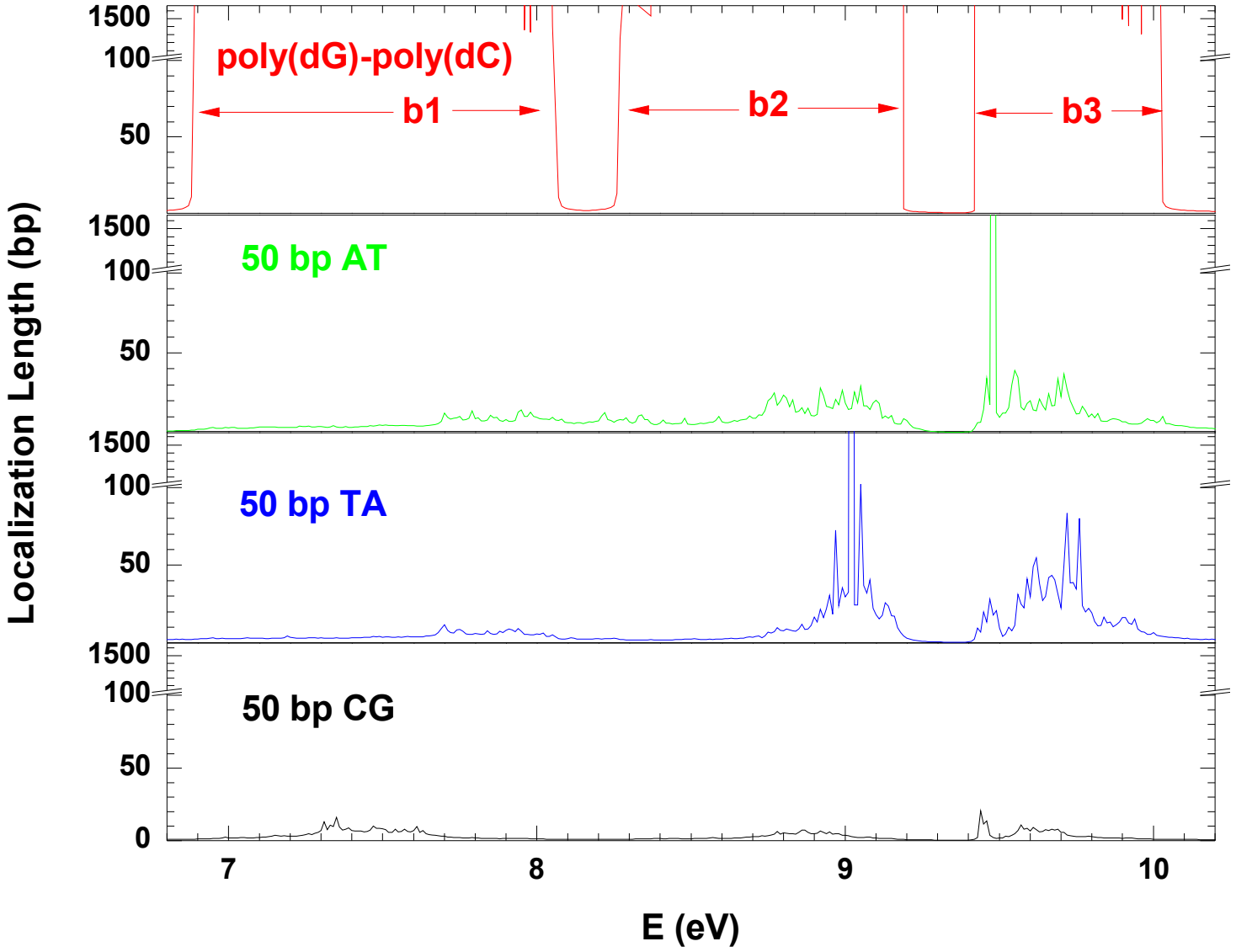
$$\gamma_{cl} = \frac{\ln\left(\prod_m \alpha_{cl}^m\right)}{2K(L-1)}$$

Ortho-normalizing

Ludlam, unpublished

Localization length=$1/\gamma_{min}$

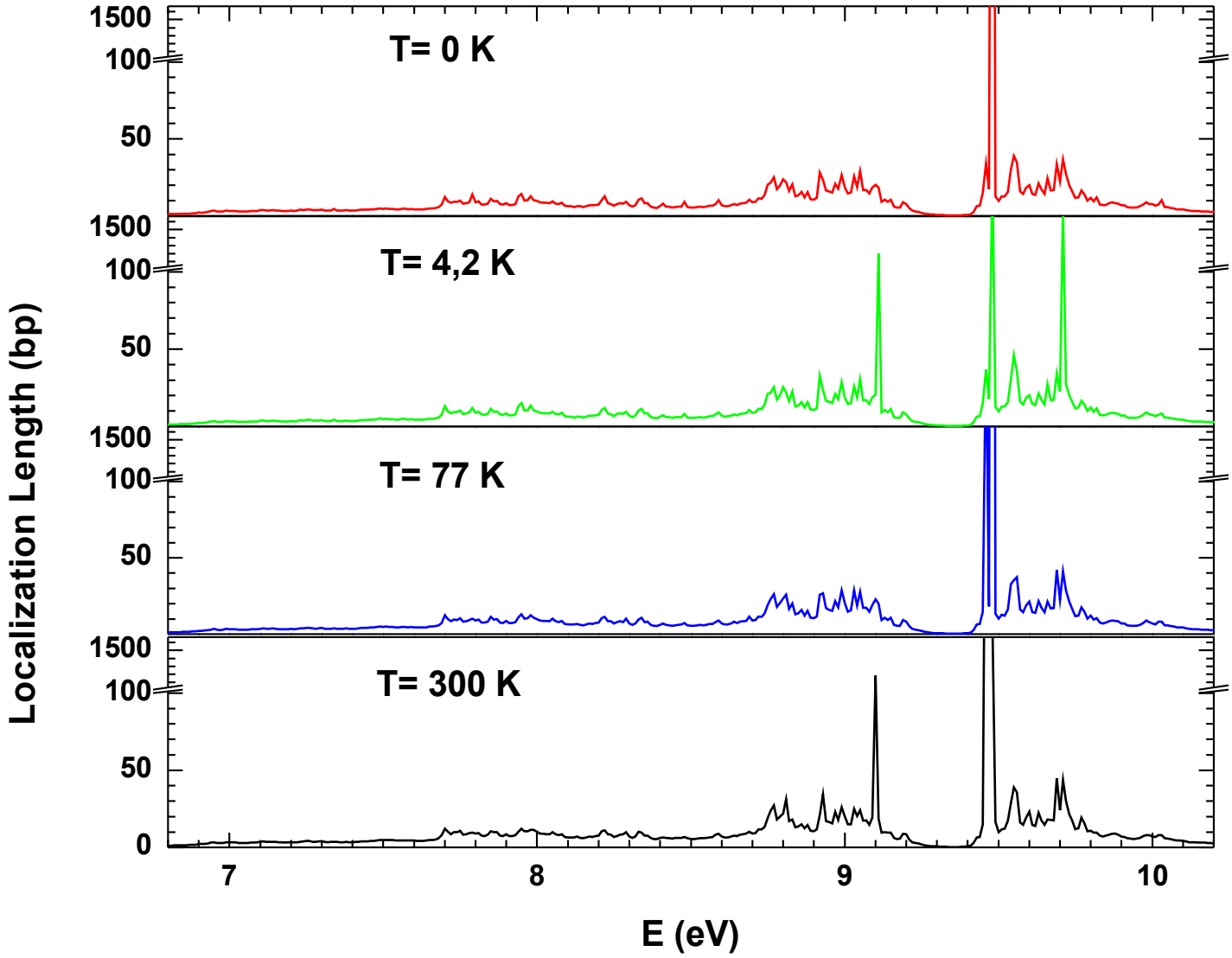
Disordered Sequence: Modified Poli(dG)-poli(dC)



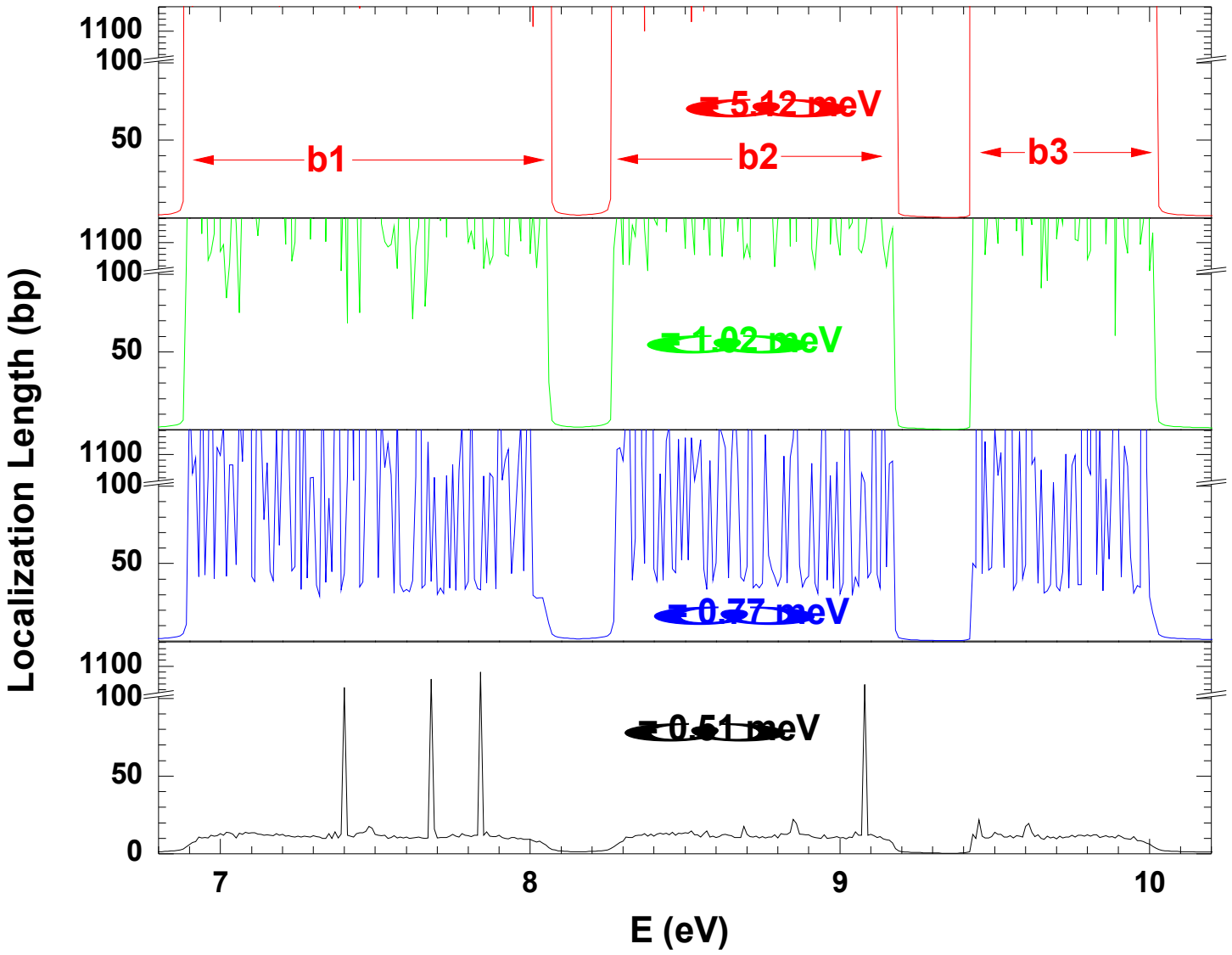
Agree with Roche, Phys. Rev. Lett.**91**, 108101 ('03) **& Klotsa *et al.*,** Biophys. J.**89,** 2187 ('05)

Temperature: Poli(dG)-poli(dC) modified with 50 bp AT

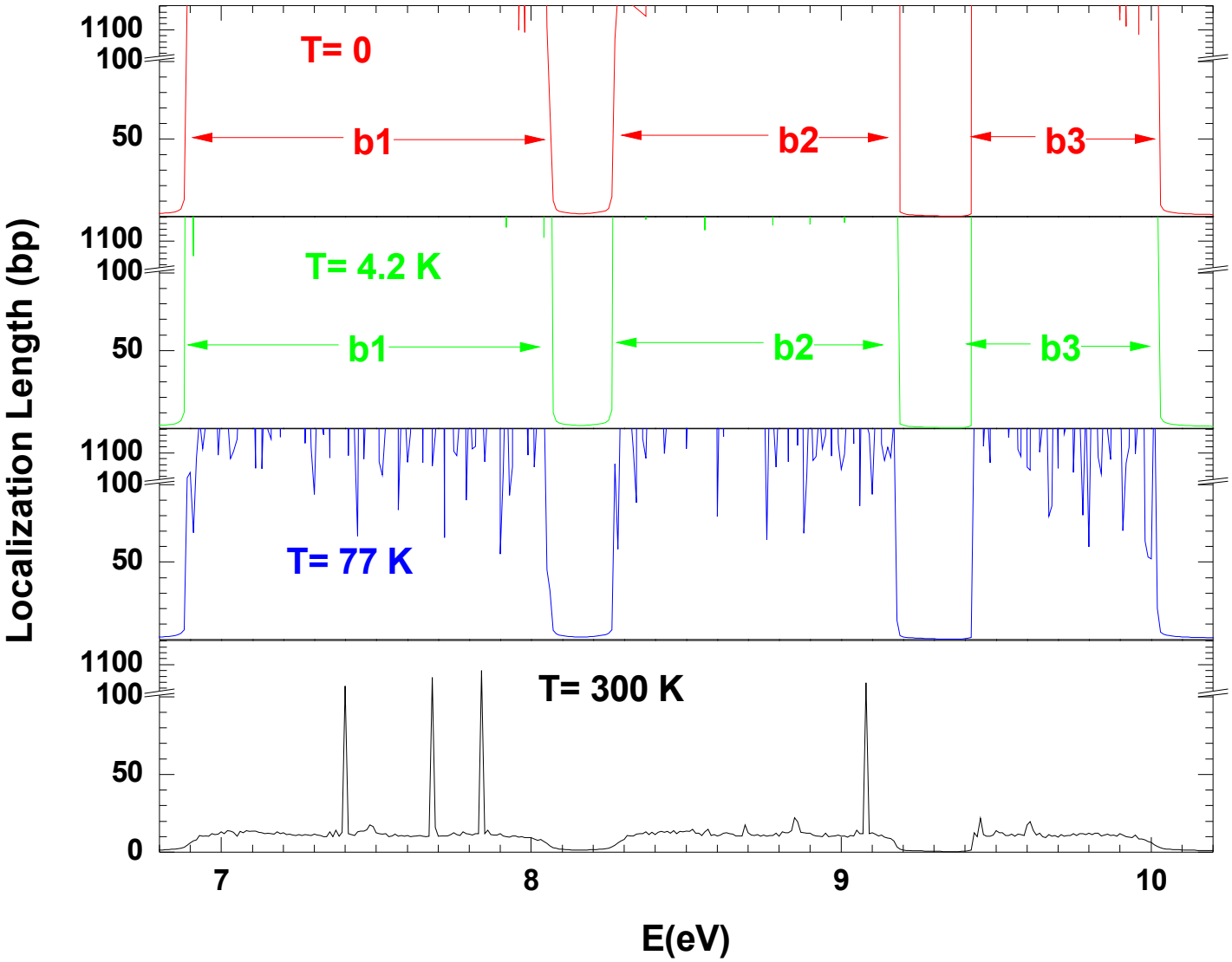
ω=5.12 meV → $\Delta\varphi$=9º at 300 K



Frequency: Poli(dG)-poli(dC) pada T=300 K



Temperature: Poli(dG)-poli(dC) at ω= 0.51 meV



Similar to Roche, Phys. Rev. Lett.**91,** 108101 ('03) **and Ren *et al.*,** Phys. Rev. B**72,** 035456 ('05)

Summary

- Disordered sequence → localized state.
- Twisting frequency 5.12 meV → little change to localization length with temperature.
- Twisting frekuensi 0.51 meV → temperature changes the localization length.
- Lower twisting frequency → lower localization length.

Phonon effects on charge transport through a DNA basepair

Efta Yudiarsah and Sergio E. Ulloa
Ohio University

Studying phonon and temperature effects on the transport through a molecule consists of two DNA bases.

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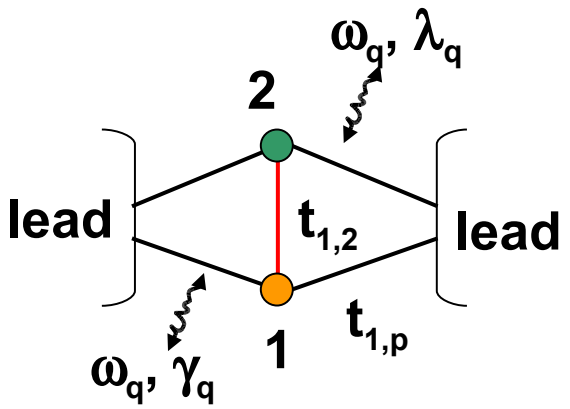
Model

- 2 States model
- Hopping between the states
- Local electron-phonon interaction
- Non-local electron-phonon interaction



States energy

Hopping

Phonon

$$H_0 = \sum_{j=1}^{2} \{\varepsilon_j c_j^+ c_j\} + t_{1,2}\left(c_1^+ c_2 + c_2^+ c_1\right) + \sum_q \omega_q a_q^+ a_q$$

$$\sum_q \left\{ \sum_{j=1}^{2} \lambda_q (a_q + a_q^+) c_j^+ c_j + \gamma_q (a_q + a_q^+)[c_1^+ c_2 + c_2^+ c_1] \right\}$$

Local

Non-local

$\omega_0 = 1meV$ Locally interact with the electron

Polaron Shift $\Delta = g\omega_0; \quad g = (\lambda_0 / \omega_0)^2$

$\omega_1 = 10meV$ Non-locally interact with the electron

Non-local electron-phonon interaction

$$\Sigma^{q}(\omega) = -\frac{1}{\beta}\sum_{m} D_q(i\omega_m) Y(\omega - i\omega_m)$$

Dressed electron Green's function

$$Y(\omega) = \begin{pmatrix} G_{22}(\omega) & G_{21}(\omega) \\ G_{12}(\omega) & G_{11}(\omega) \end{pmatrix}$$

Phonon Green's function

$$D_q(\omega)$$

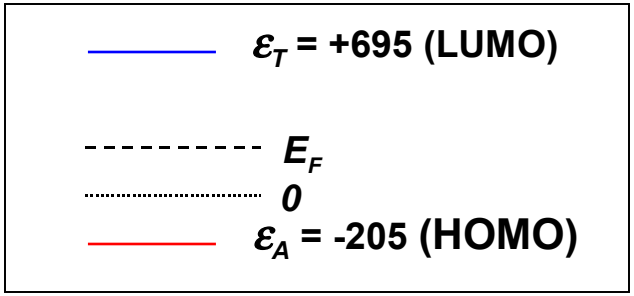
Symmetric Potential Drop at Contacts

Current: **Meir and Wingreen, PRL'92**

$$I = \frac{ie}{h}\int_{-\infty}^{+\infty} dE\, tr\left\{[\Gamma^{L} f_L(E) - \Gamma^{R} f_R(E)][G^{r}(E) - G^{r}(E)] + [\Gamma^{L} - \Gamma^{R}]G^{<}(E)\right\}$$

Used parameter

On-site energy in meV; Roche, PRL'03

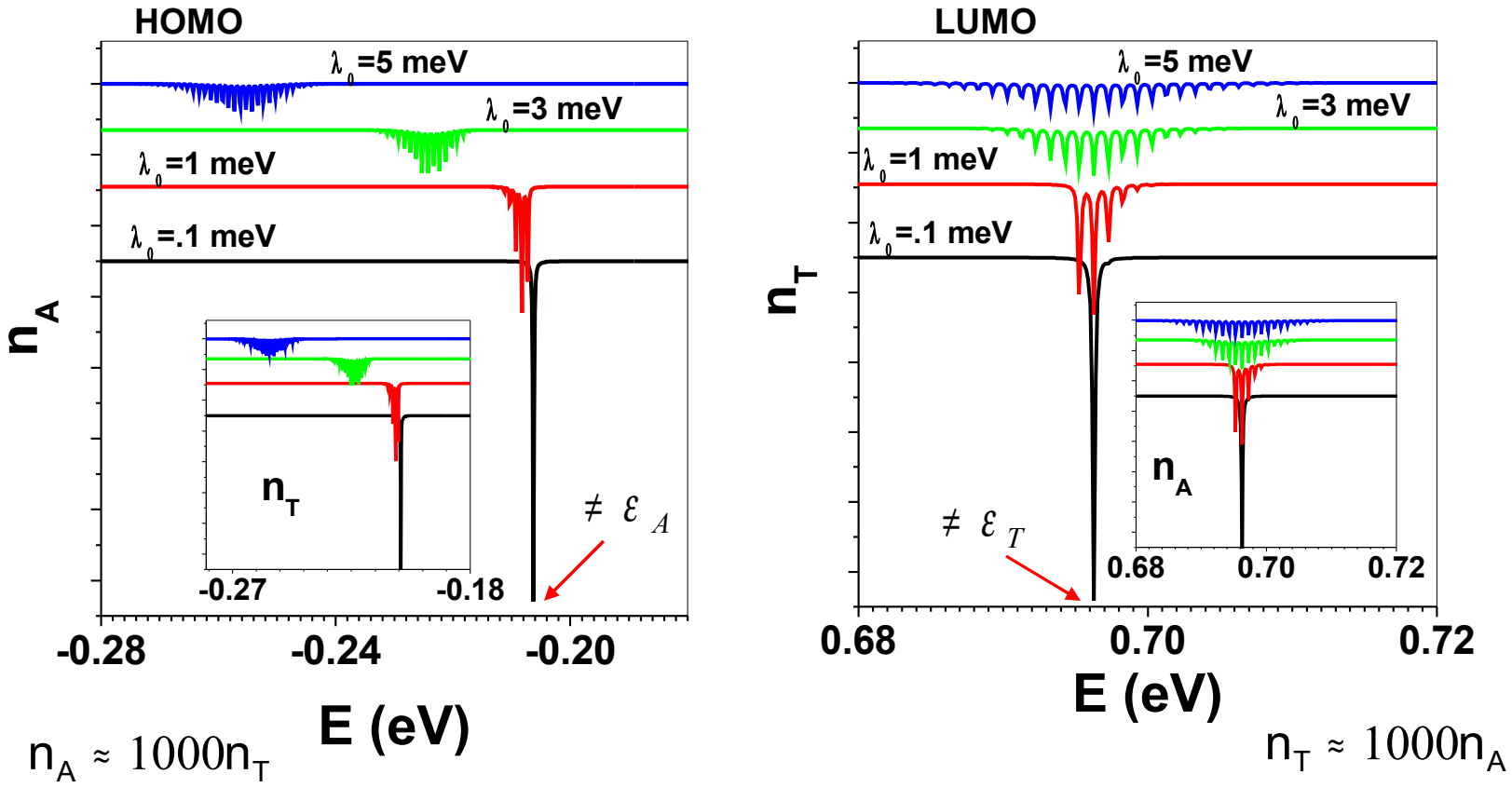


Coupling constant:

$t_{A,T}$= 34 meV; Voityuk *et al*

J Chem P '01

Polaronic Effect $T = 0K \quad \gamma_1 = .9meV$



$n_A \approx 1000 n_T$

$n_T \approx 1000 n_A$

Shifted states ⟵ **Polaron and tunneling**

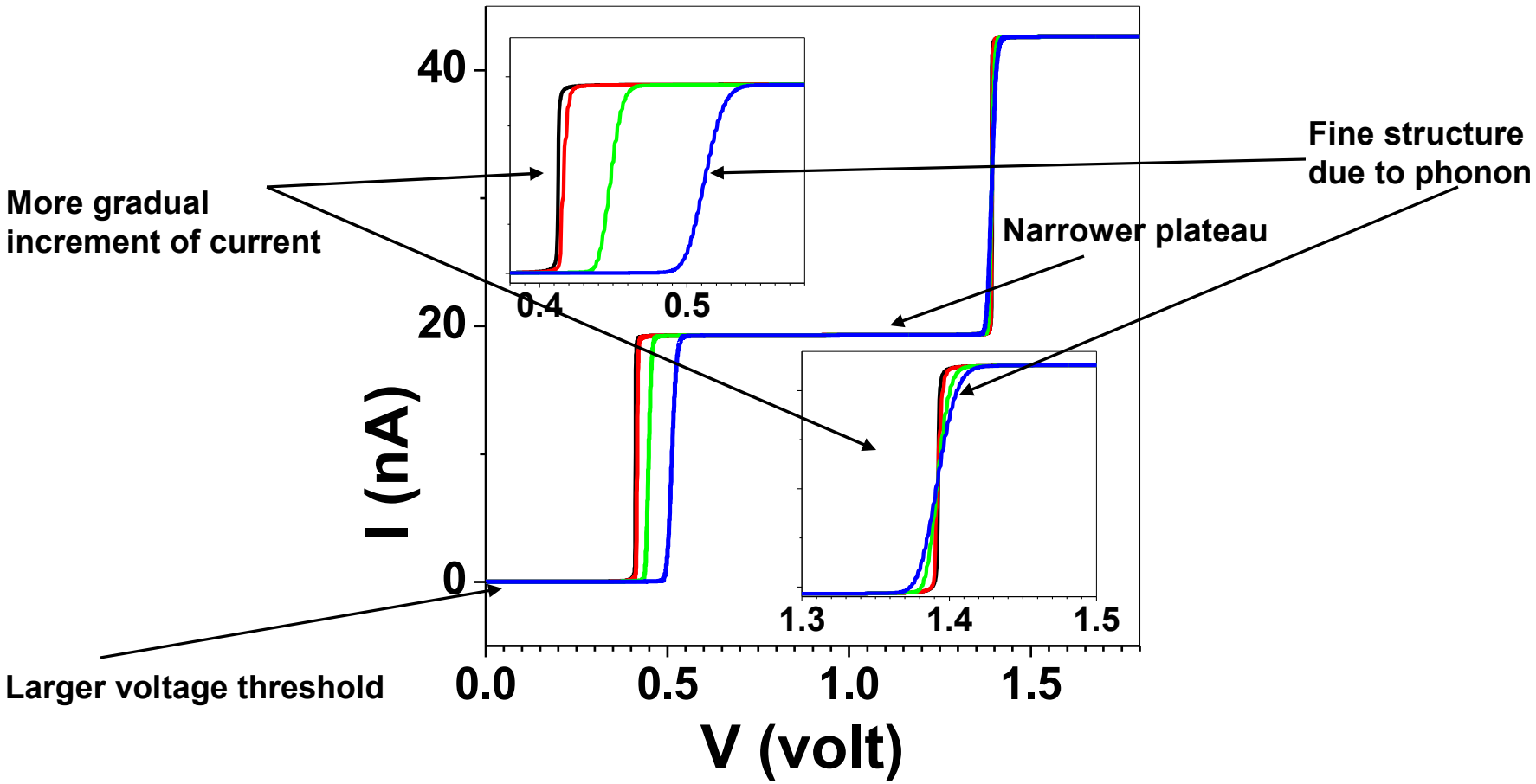
Large *g* ⟶ **larger polaron shift, more states, and lower density**

Envelope ⟶ **Poisson distribution function at low T**

Maximum Peak at

$2g\omega_0$ (HOMO) and constant (LUMO), for integer *g*

$\gamma_1 = .9meV \quad E_F = 0eV$



E_F close to HOMO ⟶ larger voltage threshold

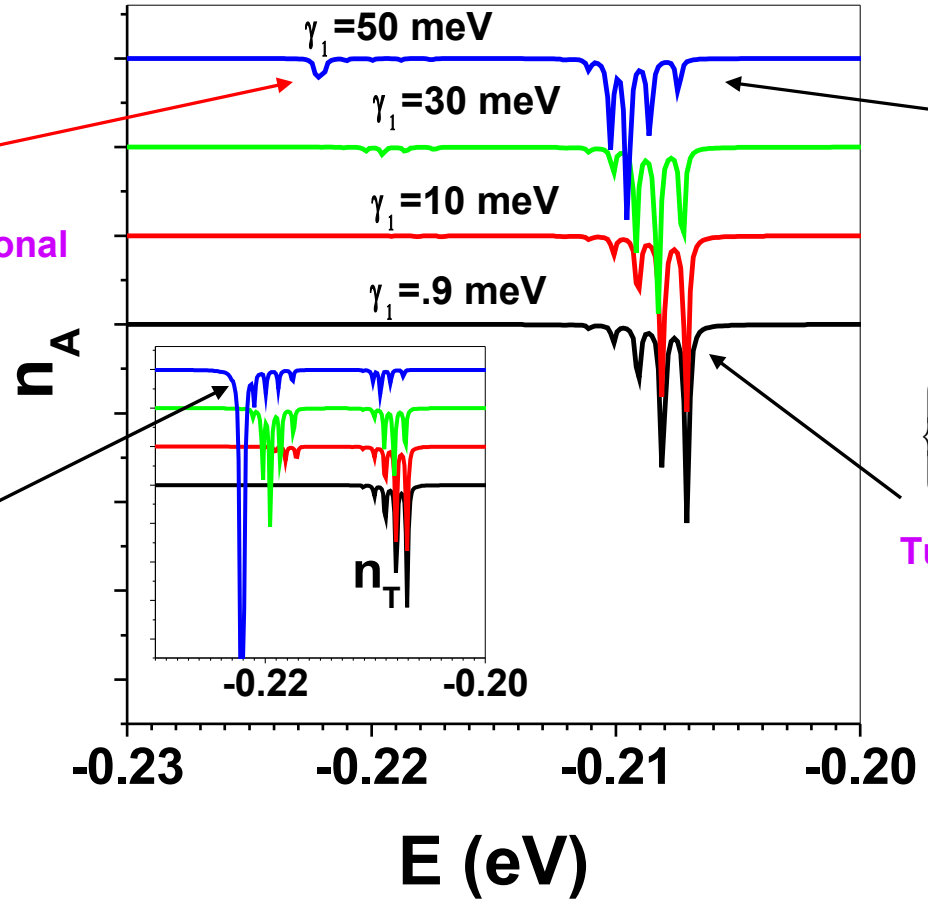
E_F close to LUMO ⟶ smaller voltage threshold

Phonon Assisted Hopping $\lambda_0 = .9meV$ $T = 0meV$

HOMO

$\left\{\frac{\gamma_1}{\omega_1}\right\}^2 > 1$

Tunneling and off-diagonal self energy effect



Satellite group lower than main group

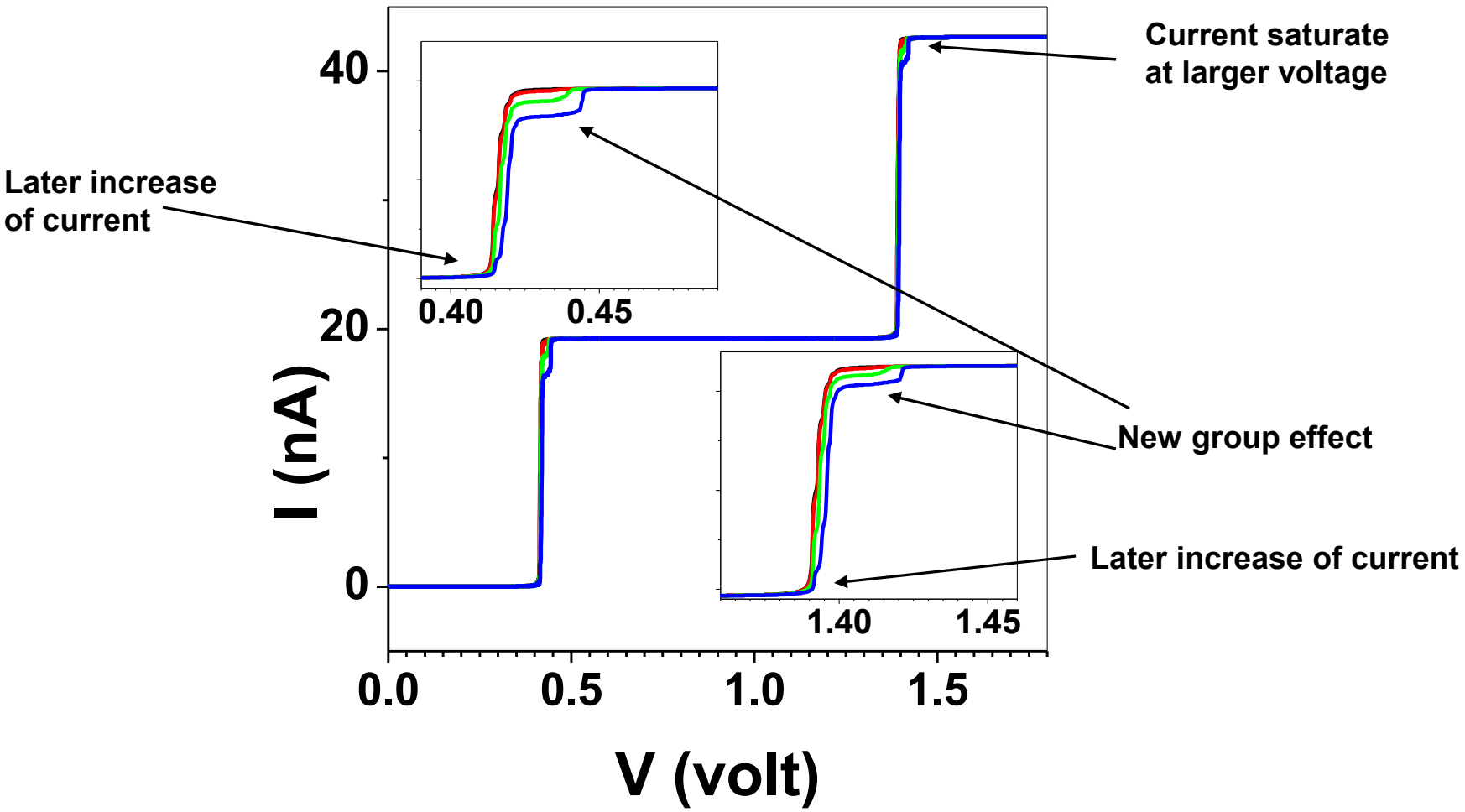
Satellite group higher than main group

$\left\{\frac{\gamma_1}{\omega_1}\right\}^2 \lesssim 1$

Tunneling and off-diagonal self energy are small

Local and non-local interaction effect on shifting and the magnitude $\gamma^2 e^{-2g}\frac{g^{l+m}}{l!m!}$

Similar trends around LUMO state, but the shift to higher energy


Current saturate
at larger voltage
Later increase
of current
New group effect
Later increase of current
40
20
0
I (nA)
0.40
0.45
1.40
1.45
0.0
0.5
1.0
1.5
V (volt)

Temperature effects $\lambda_0 = .9\text{meV}$ $\gamma_1 = 40\text{meV}$

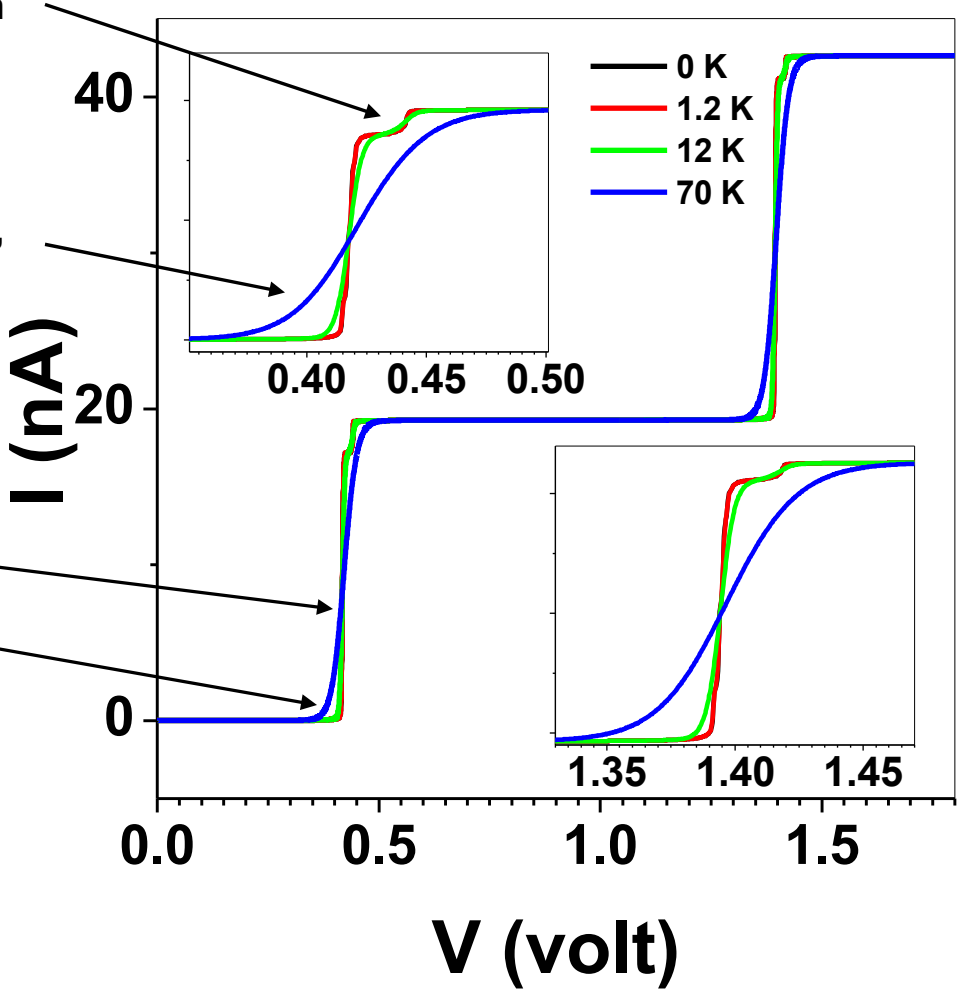
Separation of the transmission channels caused by local and non-local phonons

All fine structure is smeared out, Thermal energy > ω_0

More States

More gradual increment of current

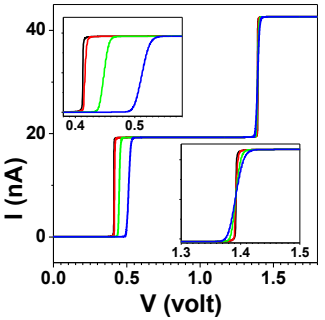
Smaller threshold



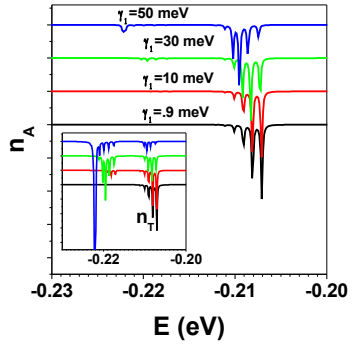
For small γ_1 a weaker effect is observed

Summary

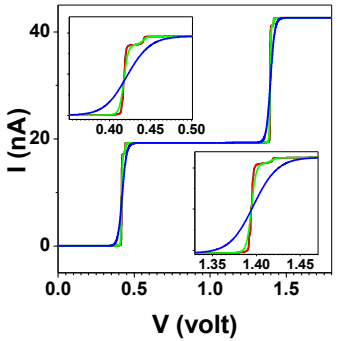
- **Local interaction creates states with smaller amplitude. Similar to the result of** Gutierrez *et al* PRB ’06 and Schmidt *et al* PRB ’07.
- **More states and gradual current increment at stronger coupling.**



- **Non-local interaction introduces new states and shifts the position of the initial states. Similar to result of** Schmidt *et al* PRB ’07.
- **More important off-diagonal self energy and the effect of coupling at stronger interaction. Non-linear effect shows up.**



- **More states, lower voltage threshold, and more gradual current increment.**



Thanks for your attention