The Abdus Salam International Centre for Theoretical Physics

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Advanced Workshop on Energy Transport in Low-Dimensional Systems: Achievements and Mysteries

15 - 24 October 2012

Heat Transport through DNA Nano-Junctions: Probing the Denaturation Transition using DNA Nonlinearity (Thermal Transport through DNA Nano-Junctions)

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Thermal transport through DNA nano-junctions

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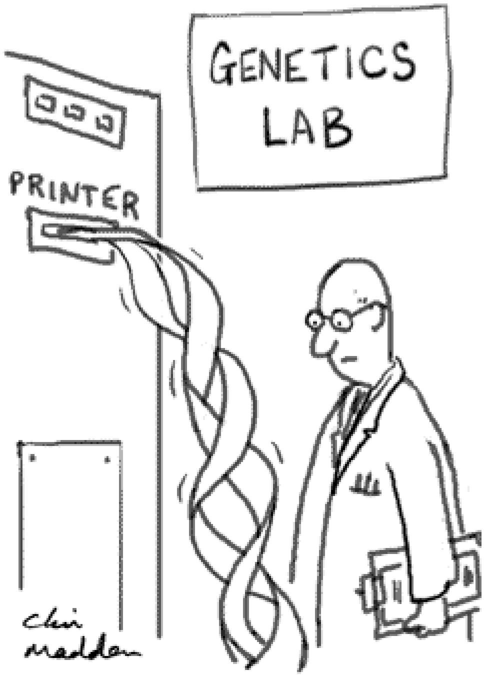
ICTP workshop: energy transport in low dimensional systems Oct. 2012

Introducing DNA



[redacted]

- A basic building-block of any life form
- Huge amount of 'know-how'
- Relevant to a large variety of disciplines:

  Physics, chemistry, biology, information science, engineering(s)

[redacted]

Basic DNA functions:

- encodes genes
- probably also other functions (junk DNA?)
- has a mechanism of reproduction

DNA reproduction:

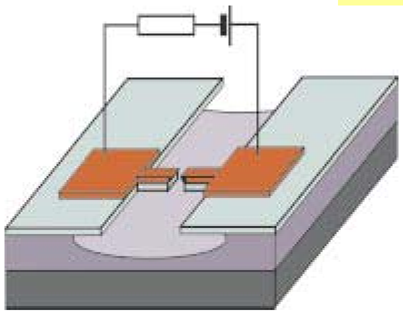
- split in two “mirror image” copies
- each copy collects its counter-part from environment

Some aspects of this process are largely unknown…

[redacted]

DNA wires

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



Special Nature Nano 2011 Focus Issue on DNA Nanotechnoloty

nature nanotechnology

REVIEW ARTICLE

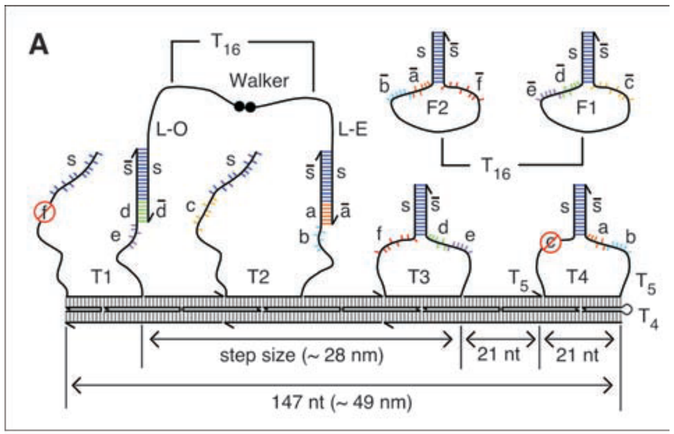
PUBLISHED ONLINE: 6 NOVEMBER 2011 | DOI: 10.1038/NNANO.2011.187

Challenges and opportunities for structural DNA nanotechnology

Andre V. Pinheiro[1], Dongran Han[1,2], William M. Shih[3,4,5*] and Hao Yan[1,2*]

DNA molecules have been used to build a variety of nanoscale structures and devices over the past 30 years, and potential applications have begun to emerge. But the development of more advanced structures and applications will require a number of issues to be addressed, the most significant of which are the high cost of DNA and the high error rate of self-assembly. Here we examine the technical challenges in the field of structural DNA nanotechnology and outline some of the promising applications that could be developed if these hurdles can be overcome. In particular, we highlight the potential use of DNA nanostructures in molecular and cellular biophysics, as biomimetic systems, in energy transfer and photonics, and in diagnostics and therapeutics for human health.

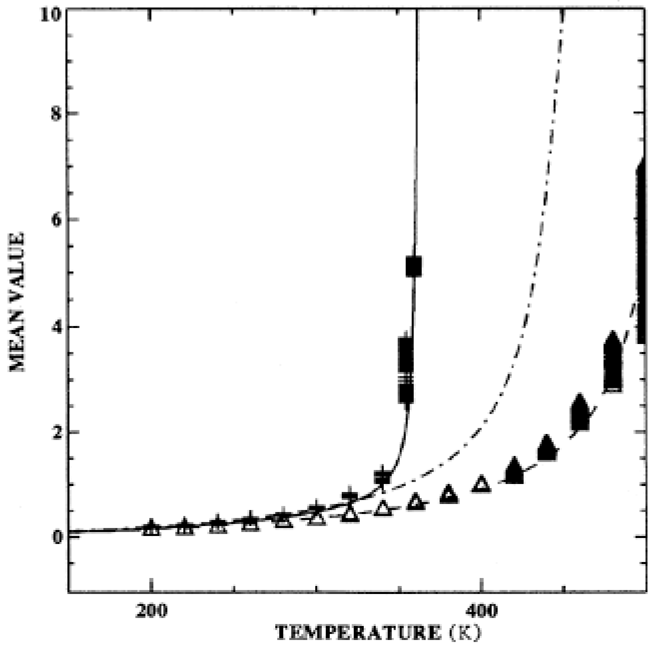
DNA motors



[omabegho *et al.*, Science **324**, 67(2009)]

DNA Denaturation transition

DNA denaturates at ~350K



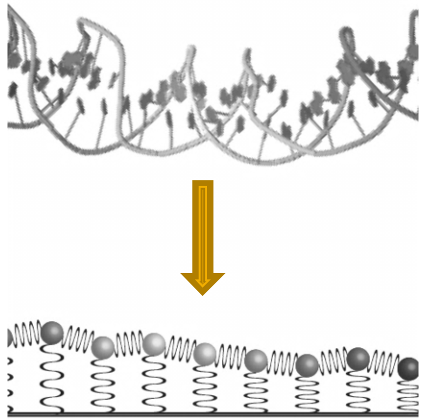
Interplay of thermal fluctuations and non-linear interactions

http://www.youtube.com/watch?v=dnhZ5jEv_9I

DNA Denaturation transition

"The standard Model"

M. Peyrard and A. R. Bishop, Phys. Rev. Lett. 62, 2755 (1989).
T. Dauxois, M. Peyrard, and A. R. Bishop, Phys. Rev. E 47, R44 (1993).



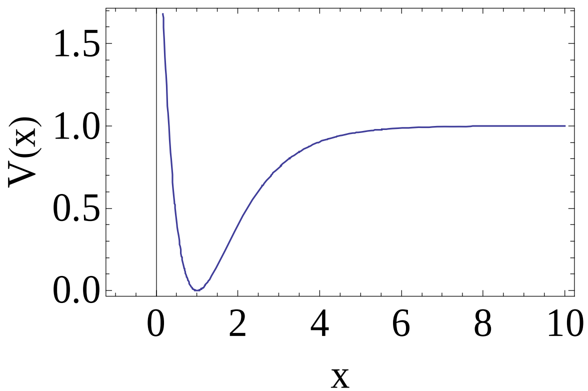
$$H = \sum_n \left[\frac{m\dot{y}_n^2}{2} + V\left(y_n\right) + W\left(y_n, y_{n-1}\right) \right]$$

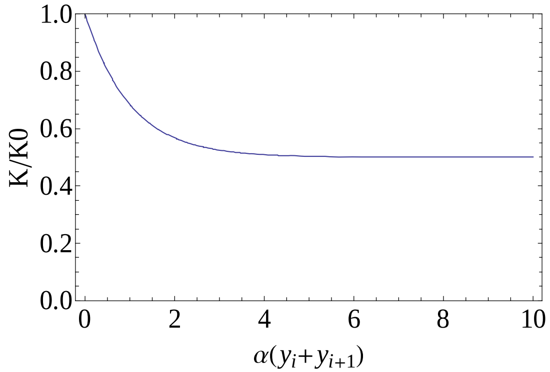
$$V(y_n) = D(e^{-ay_n} - 1)^2$$

Single-Pair Potential

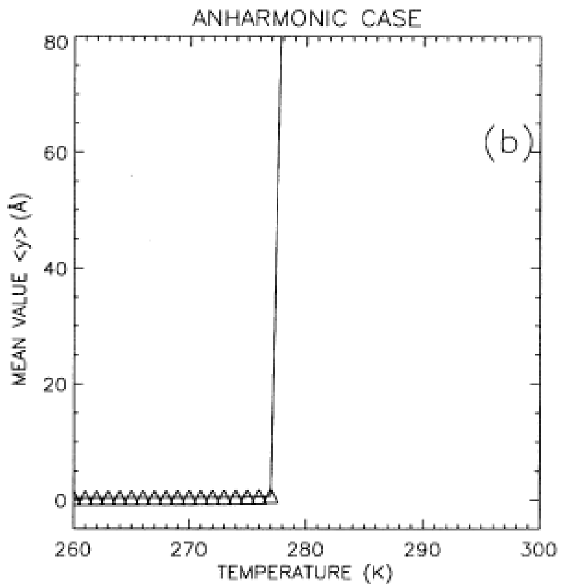
$$W(y_n, y_{n-1}) = (K/2)(1 + \rho e^{-\alpha(y_n + y_{n-1})})(y_n - y_{n-1})^2$$

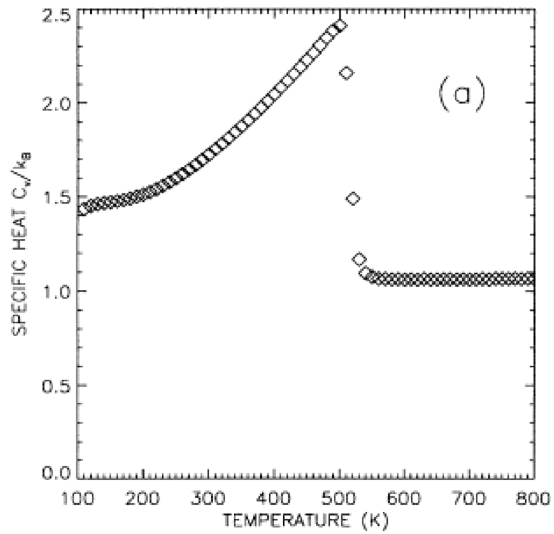
Pair-Pair Interaction



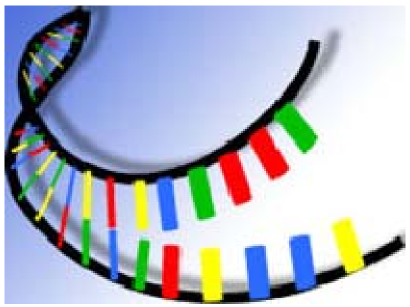


DNA Denaturation transition





T. Dauxois, M. Peyrard, Phys. Rev. E 51, 4027 (1995).



Conditions for transition:

1. Plateau in Morse potential
2. Strong Non-linearity: K decrease with increase $\langle y \rangle$

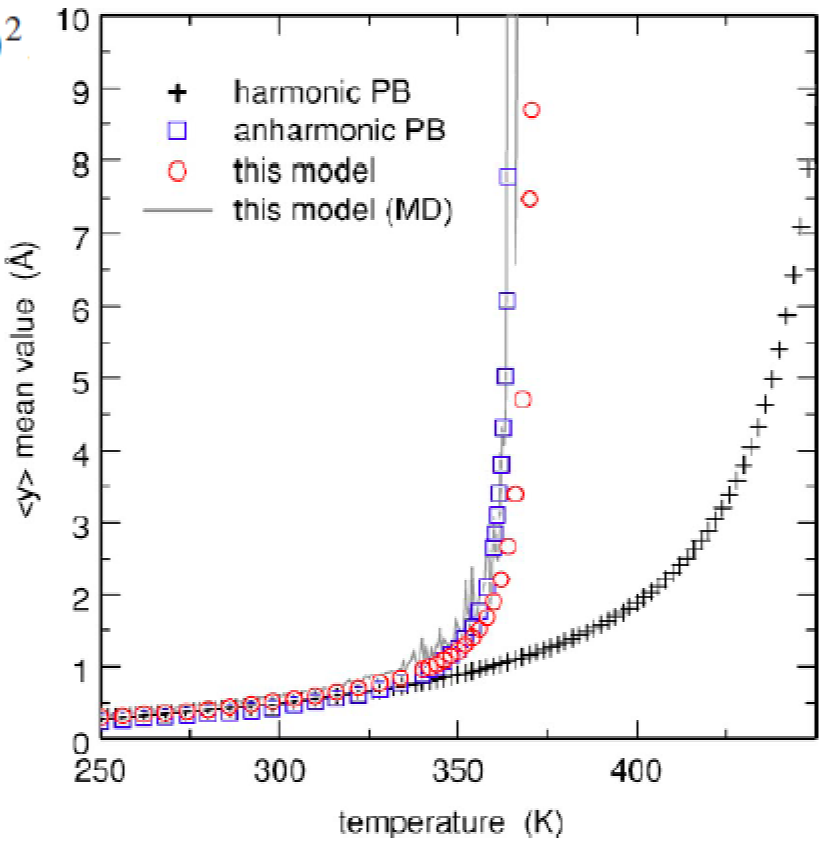
T. Dauxois, M. Peyrard, Mathematics and Computers in Simulation **40**, 305 (1996).

DNA Denaturation transition

BUT…
Different models (with different interactions) give same denaturation transition

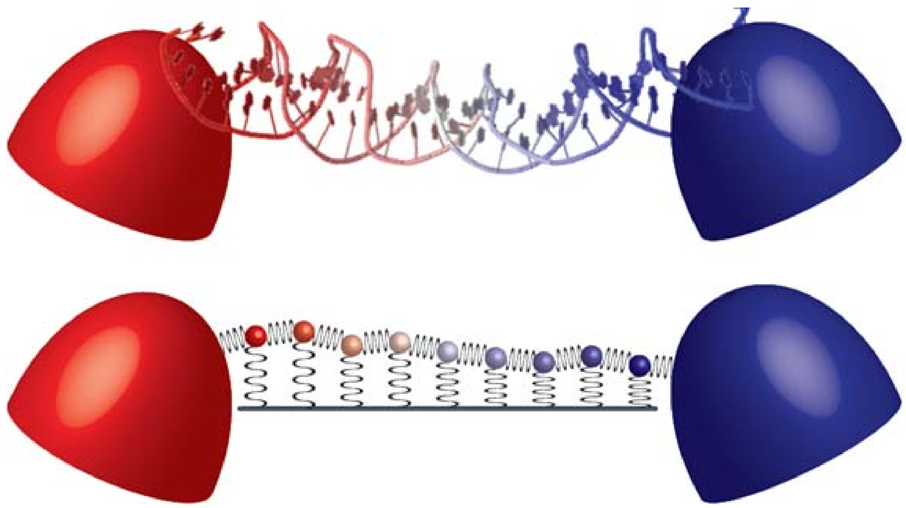
$$W(y_n, y_{n+1}) = \frac{\Delta H}{2}\left(1 - e^{-b(y_n - y_{n+1})^2}\right) + K_b(y_n - y_{n+1})^2$$

M. Joyeux and S. Buyukdagli
PRE 72, 51902 (2005)



DNA Denaturation transition

- How can one distinguish between the two models?
- What are the signatures of the non-linearities?
- Can DNA be used as a thermal device?



Thermal conductivity across the DNA Denaturation transition

Calculating the thermal conductivity :

Step I: Harmonic limits

	High-T	Low-T
PBD	$D_H = 0, K_H = K$	$D_L = Da^2, K_L = K(1+\rho)$
JB	$D_L = 0, K_L = K_b$	$D_L = Da^2, K_L = K_b + \frac{b\Delta H}{2}$

$K = 0.04\ eV/Å^2$

$K_b = 10^{-5}\ eV/Å^2 \quad \Delta H = 0.44\ eV,\ b = 0.1Å^{-2}$

Thermal conductivity across the DNA Denaturation transition

Calculation of thermal conductance: Harmonic chain approximation

$$m\ddot{y}_n \;=\; -2(D_\mu + K_\mu)y_n + K_\mu(y_{n-1} + y_{n+1}) + (\delta_{n,1} + \delta_{n,N})\left[-\gamma\dot{y}_n(t) + \eta_n(t)\right].$$

$$y_n(t) = (1/2\pi)\int^{\infty} d\omega \hat{Y}^{-1}_{nm}(\omega)\hat{\eta}_m(\omega)e^{i\omega t}$$

$$J_\mu \;=\; \frac{\Delta T\lambda^2 m^2}{\pi}\int_{-\infty}^{\infty} d\omega\omega^2\{(\mathcal{D}_{1,N} - \lambda^2\omega^2 m^2\mathcal{D}_{2,N-1})^2\ \lambda^2\omega^2 m^2(\mathcal{D}_{1,N-1} + \mathcal{D}_{2,N})^2\}^{-1}|C_{1,N}|^2$$

$$\frac{J_\mu}{\Delta T} = \frac{\gamma}{2\pi m}\int_0^{2\pi} dq \frac{\sin^2(q)}{1 + \frac{2\gamma^2}{mK_\mu}\left[1 + \frac{D_\mu}{K_\mu} - \cos(q)\right]}.$$

$$\kappa_\mu = \frac{k_B m K_\mu^2}{4\gamma^3}\left[1 + \frac{2\gamma^2}{mK_\mu} + \frac{2\gamma^2 D_\mu}{mK_\mu^2} - \mathcal{B}_\mu\right],$$

$$\mathcal{B}_\mu = \sqrt{1 + \frac{4\gamma^2}{mK_\mu} + \frac{4\gamma^2 D_\mu}{mK_\mu^2} + \frac{8\gamma^4 D_\mu}{m^2K_\mu^3} + \frac{4\gamma^4 D_\mu^2}{m^2K_\mu^4}}.$$

Casher and Lebowitz,
Journal of Mathematical Physics **12**, 1701 (1971)

Thermal conductivity across the DNA Denaturation transition

Numerical Simulation: Langevin Equation (tests also with Nose-Hoover bath)

$$m\ddot{y}_n = -\frac{\partial W}{\partial y_n} - \frac{\partial V}{\partial y_n} - \Gamma_n \dot{y}_n + f(t)$$

$D = 0.04\,\mathrm{eV}$

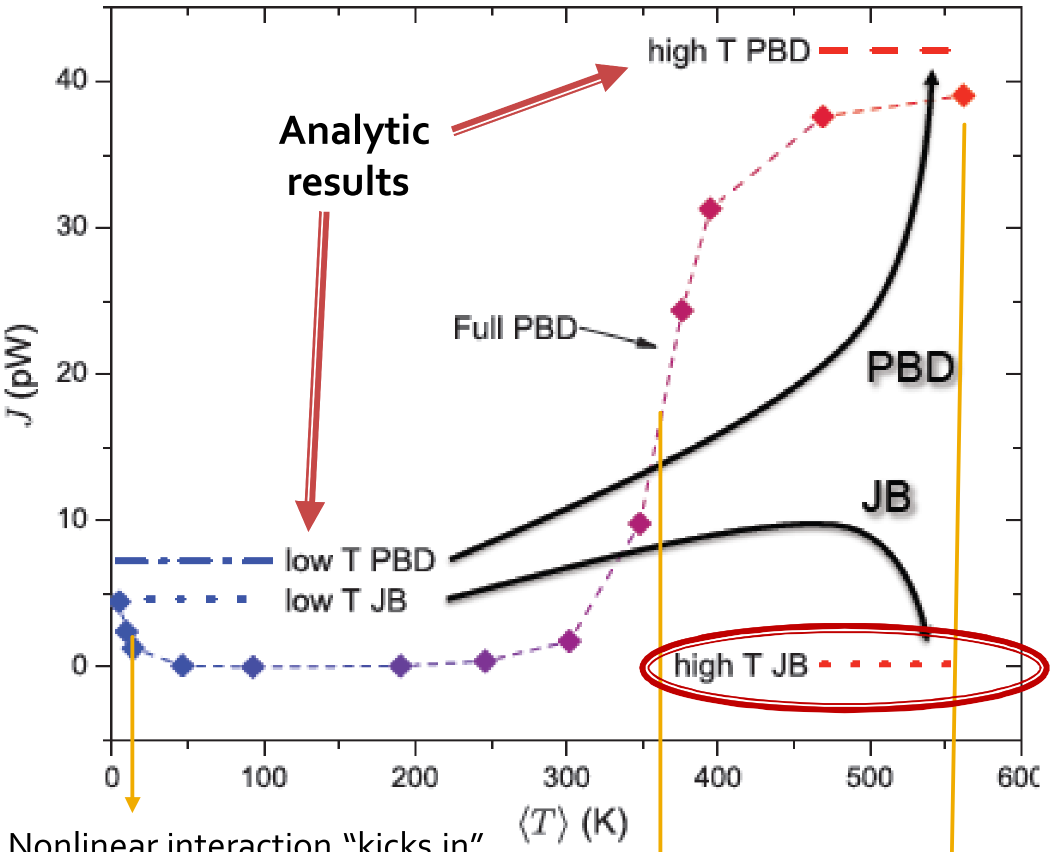
$a = 4.47\,\mathrm{\AA}^{-1}$

$K = 0.04\,\mathrm{eV}/\mathrm{\AA}^2$

$\rho = 0.5$

$\alpha = 0.358\,\mathrm{\AA}^{-1}$

Thermal conductivity across the DNA Denaturation transition

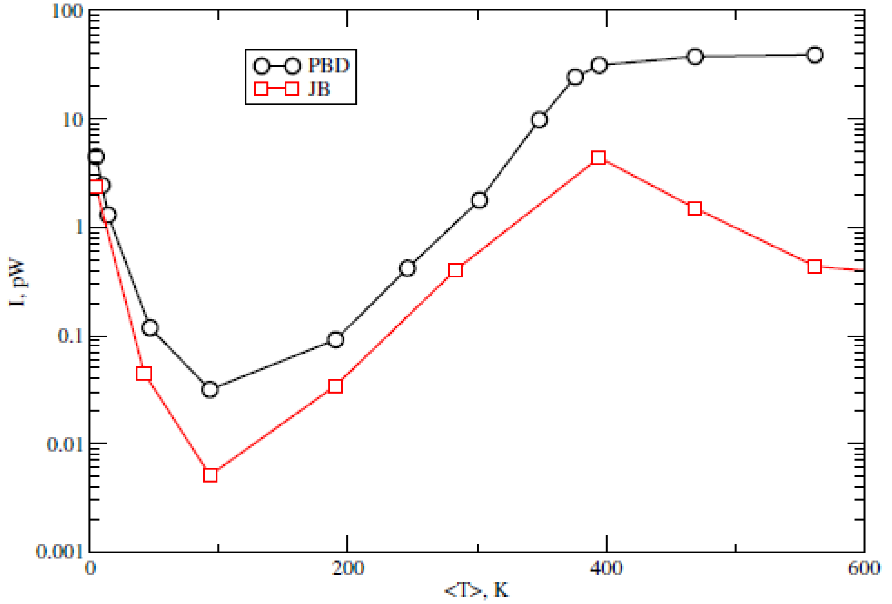


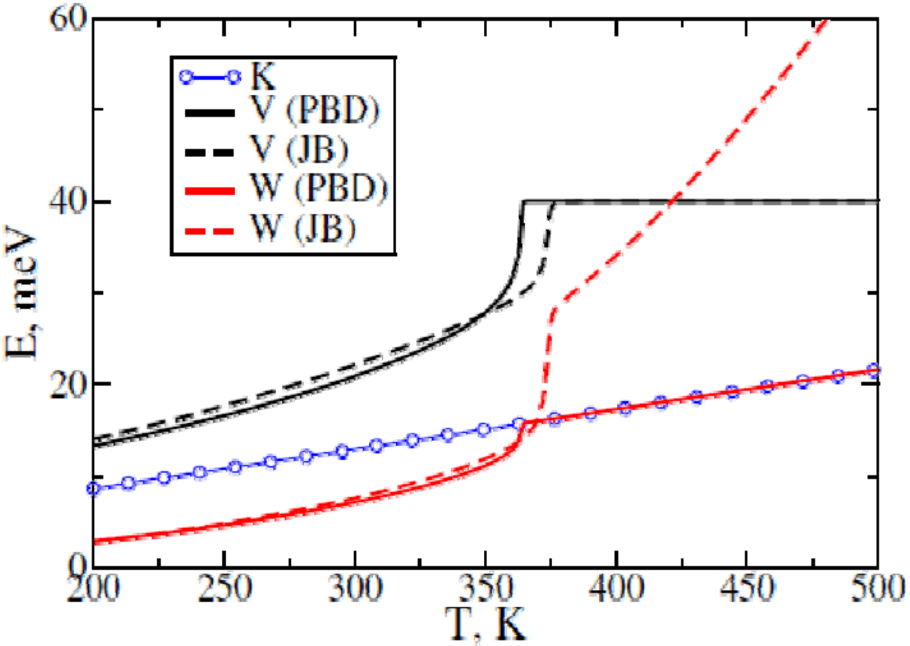
Nonlinear interaction "kicks in"

Strand separation

"softening" of the chain upon denaturation

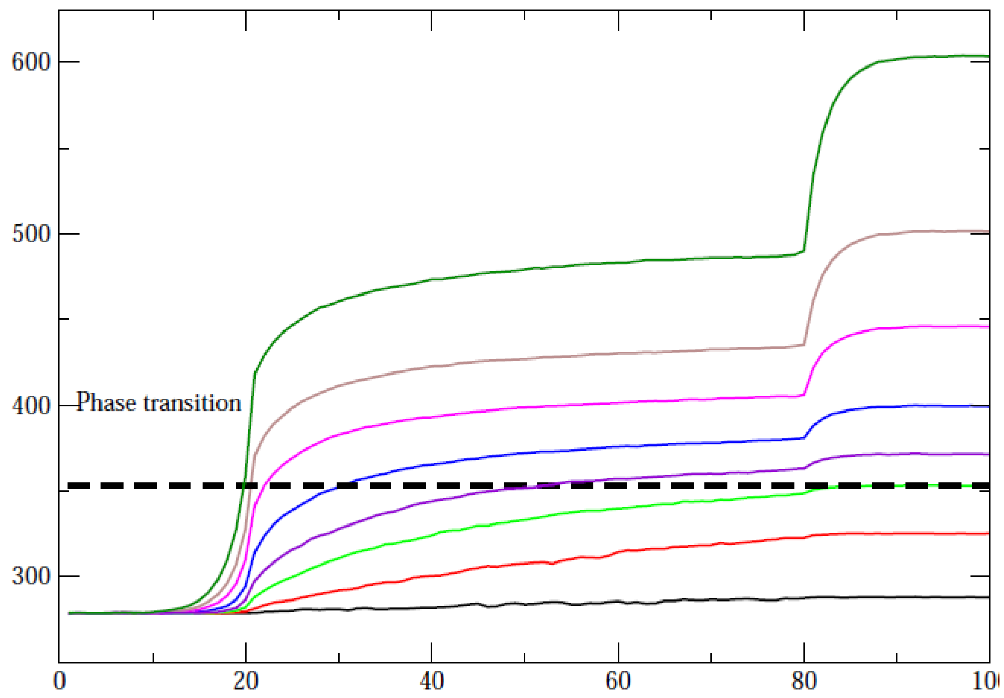
Thermal conductivity across the DNA Denaturation transition



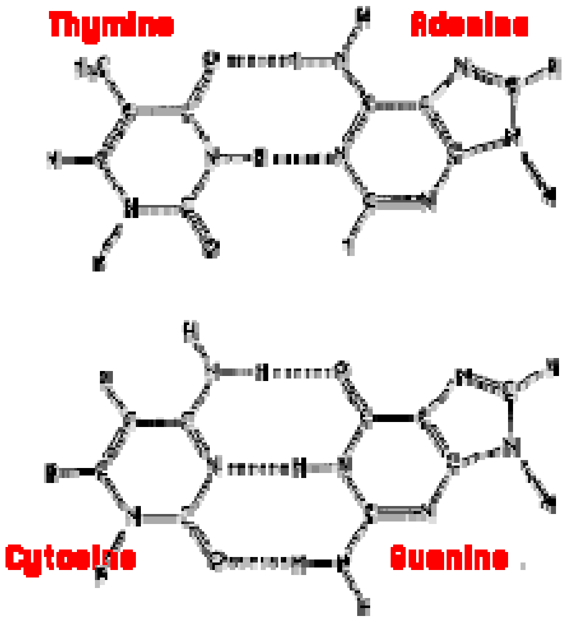


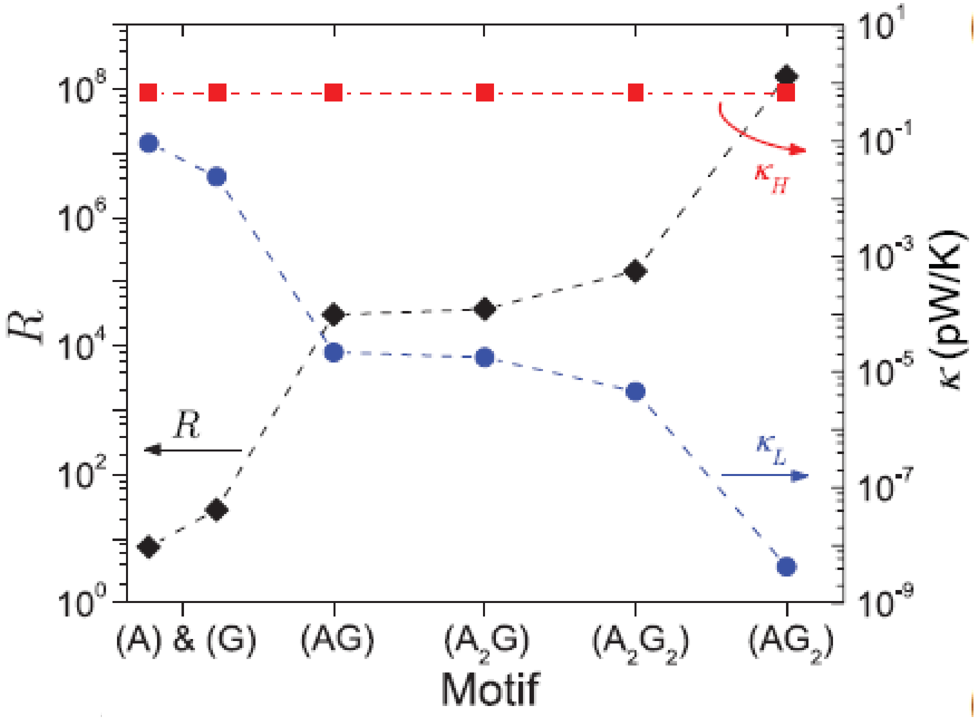
Thermal conductivity across the DNA Denaturation transition

Local temperature $T_n = \frac{1}{2} m \langle \dot{y}_n^2 \rangle$

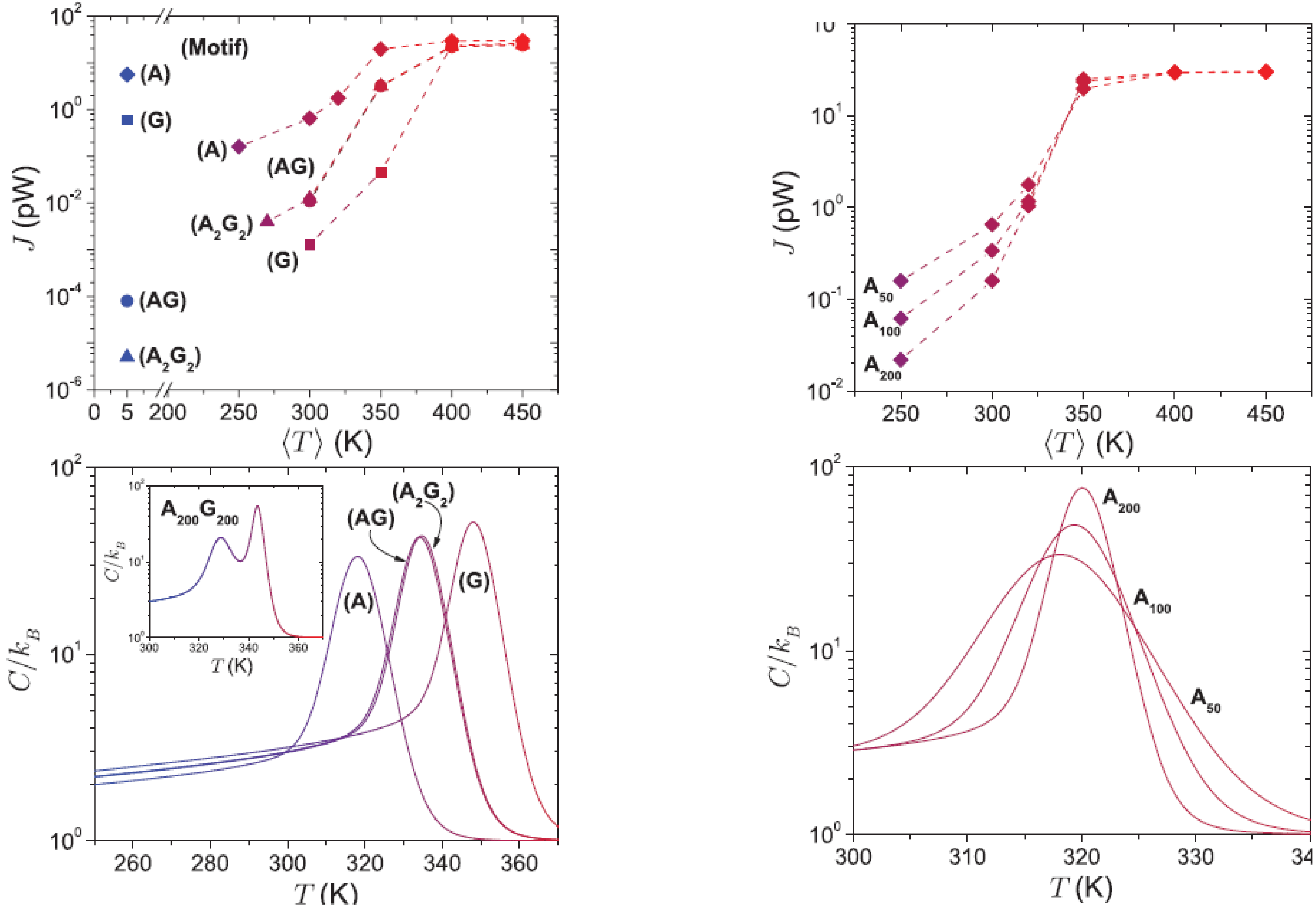


Engineering DNA thermal switching



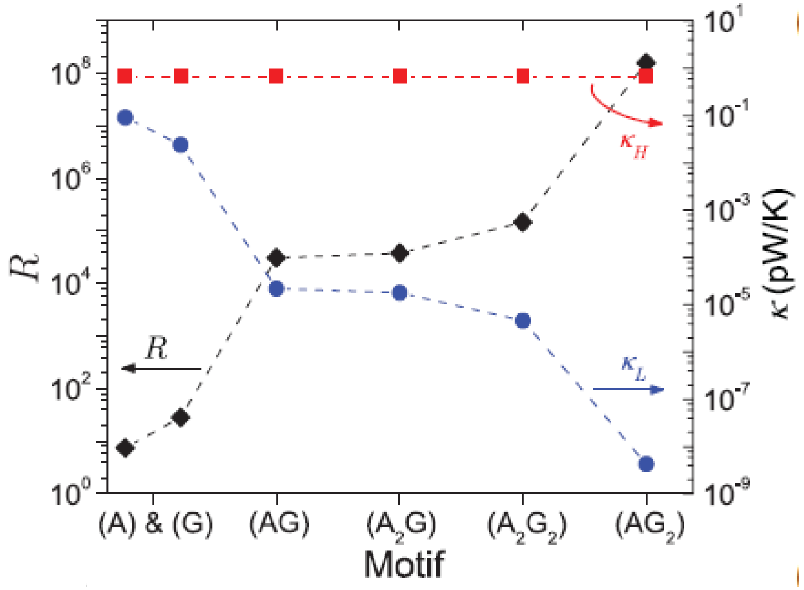


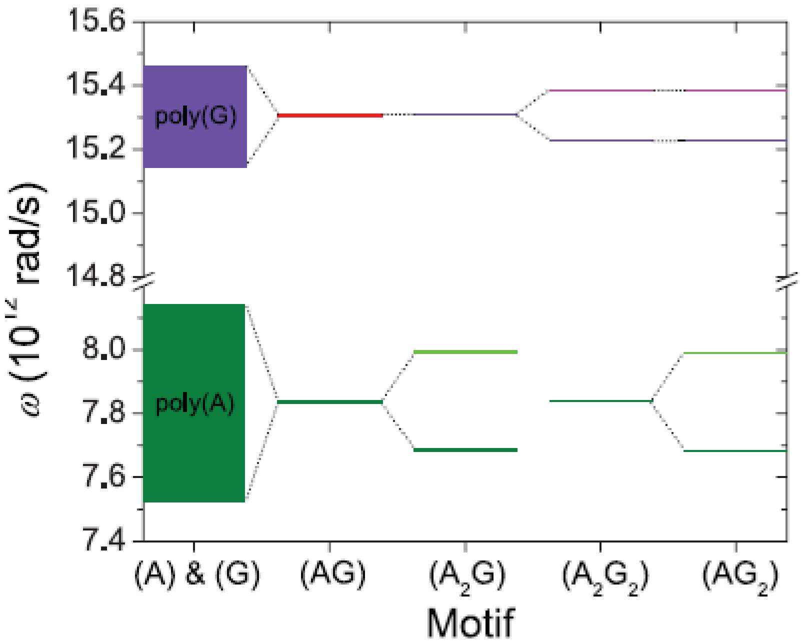
Engineering DNA thermal switching



Engineering DNA thermal switching

Origin of difference at low T: phonon bands





Engineering DNA thermal switching

Remark: Thermal current and phonon group velocity

Lebowitz-Casher Formula:

$$J = \frac{\gamma}{\pi K} \int_W d\omega\omega \frac{|\sin q|}{1 + \frac{2\gamma^2}{mK}(1 + \frac{D}{K} - \cos q)} \Delta T$$

$m\omega^2 = 2(K + D) - 2K \cos q$ so that $\frac{d\omega}{dq} = \frac{K}{m\omega} \sin q$

In the large γ limit $\gamma^2/(mK) \gg 1$

$$J \approx \frac{\gamma}{2\pi K} \int_W d\omega\omega \frac{\frac{m\omega}{K} \frac{d\omega}{dq}}{\frac{2\gamma^2}{mK} m\omega^2} \Delta T = \frac{m}{2\pi\gamma} \int_W d\omega \frac{d\omega}{dq} \Delta T$$

Engineering DNA thermal switching

In the two-band (A-G) case: $[x_1][x_2] - 2 = 2\cos q,$

$[x_1] = 2(1 + D_1/K) - m\omega^2/K$ and $[x_2] = 2(1 + D_2/K) - m\omega^2/K$

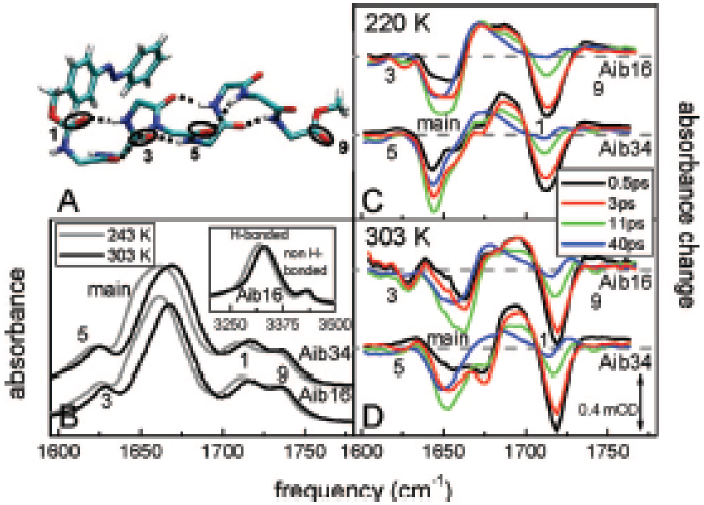
Defines the group velocity

$$-2\sin q = \frac{d[x_1]}{dq}[x_2] + \frac{d[x_2]}{dq}[x_1] = -2\frac{m}{K}\omega\frac{d\omega}{dq}([x_1] + [x_2]).$$

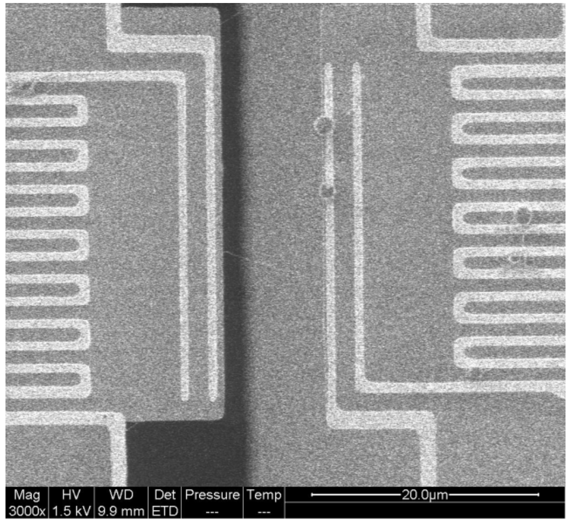
And again for large γ we get

$$\begin{aligned}
\frac{J}{\Delta T} &= \frac{m\gamma}{\pi K^2}\int_W d\omega\omega|\sin q|[(1 + \gamma^2\omega^2/K^2) \times \\
&\quad (m/K)([x_1] + [x_2])]^{-1} \\
&\approx \frac{m\gamma}{\pi K^2}\int_W d\omega\omega\frac{|\sin q|}{\frac{\gamma^2\omega^2}{K^2}\frac{m}{K}([x_1] + [x_2])} \\
&= \frac{m\gamma}{\pi K^2}\int_W d\omega\omega\frac{\frac{m}{K}\omega\frac{d\omega}{dq}([x_1] + [x_2])}{\frac{\gamma^2\omega^2}{K^2}\frac{m}{K}([x_1] + [x_2])} \\
&= \frac{m}{\pi\gamma}\int_W d\omega\frac{d\omega}{dq}.
\end{aligned}$$

Measuring DNA thermal conductivity

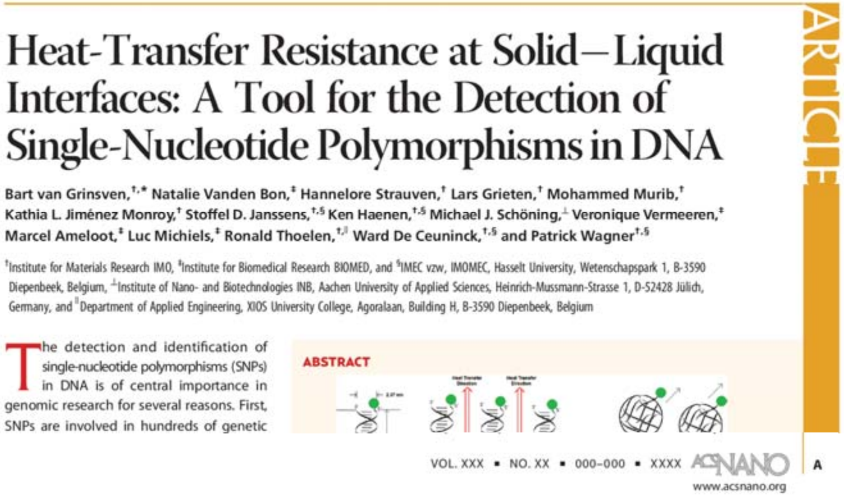


Backus *et al.*,
J. Phys. Chem. B, **112**, 15487 (2008)



R. Chen
Private communication

Measuring DNA thermal conductivity



ARTICLE

Heat-Transfer Resistance at Solid–Liquid Interfaces: A Tool for the Detection of Single-Nucleotide Polymorphisms in DNA

Bart van Grinsven,[†,*] Natalie Vanden Bon,[‡] Hannelore Strauven,[†] Lars Grieten,[†] Mohammed Murib,[†] Kathia L. Jiménez Monroy,[†] Stoffel D. Janssens,[†,§] Ken Haenen,[†,§] Michael J. Schöning,[⊥] Veronique Vermeeren,[‡] Marcel Ameloot,[‡] Luc Michiels,[‡] Ronald Thoelen,[†,∥] Ward De Ceuninck,[†,§] and Patrick Wagner[†,§]

[†]Institute for Materials Research IMO, [‡]Institute for Biomedical Research BIOMED, and [§]IMEC vzw, IMOMEC, Hasselt University, Wetenschapspark 1, B-3590 Diepenbeek, Belgium, [⊥]Institute of Nano- and Biotechnologies INB, Aachen University of Applied Sciences, Heinrich-Mussmann-Strasse 1, D-52428 Jülich, Germany, and [∥]Department of Applied Engineering, XIOS University College, Agoralaan, Building H, B-3590 Diepenbeek, Belgium

The detection and identification of single-nucleotide polymorphisms (SNPs) in DNA is of central importance in genomic research for several reasons. First, SNPs are involved in hundreds of genetic

ABSTRACT

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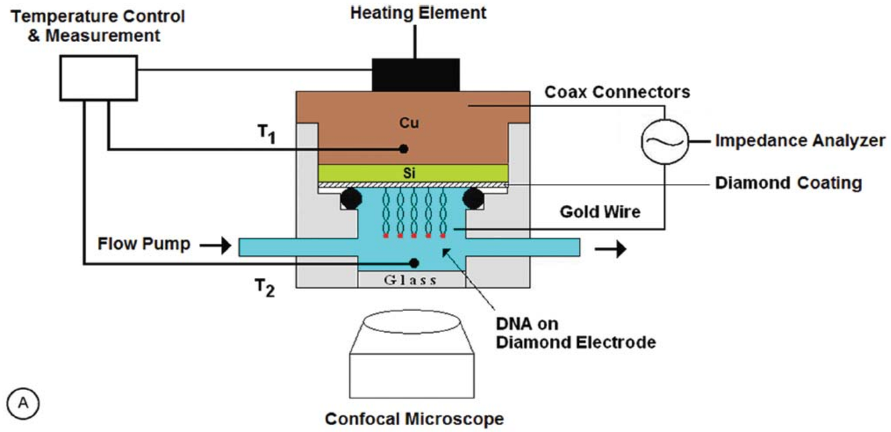
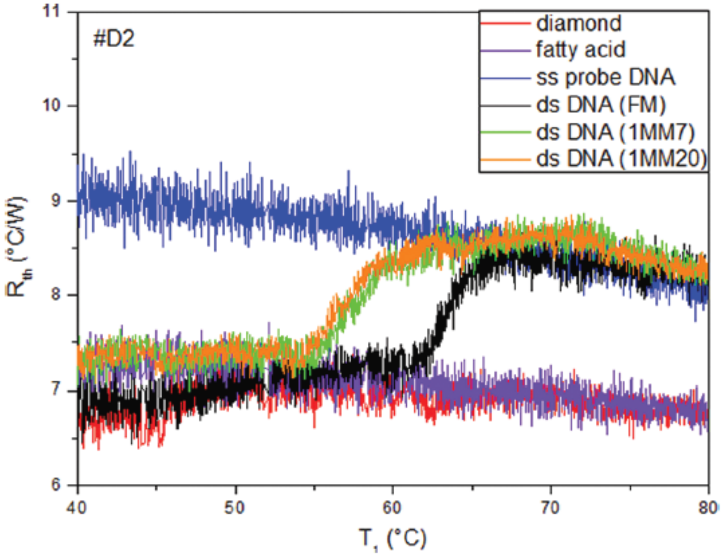
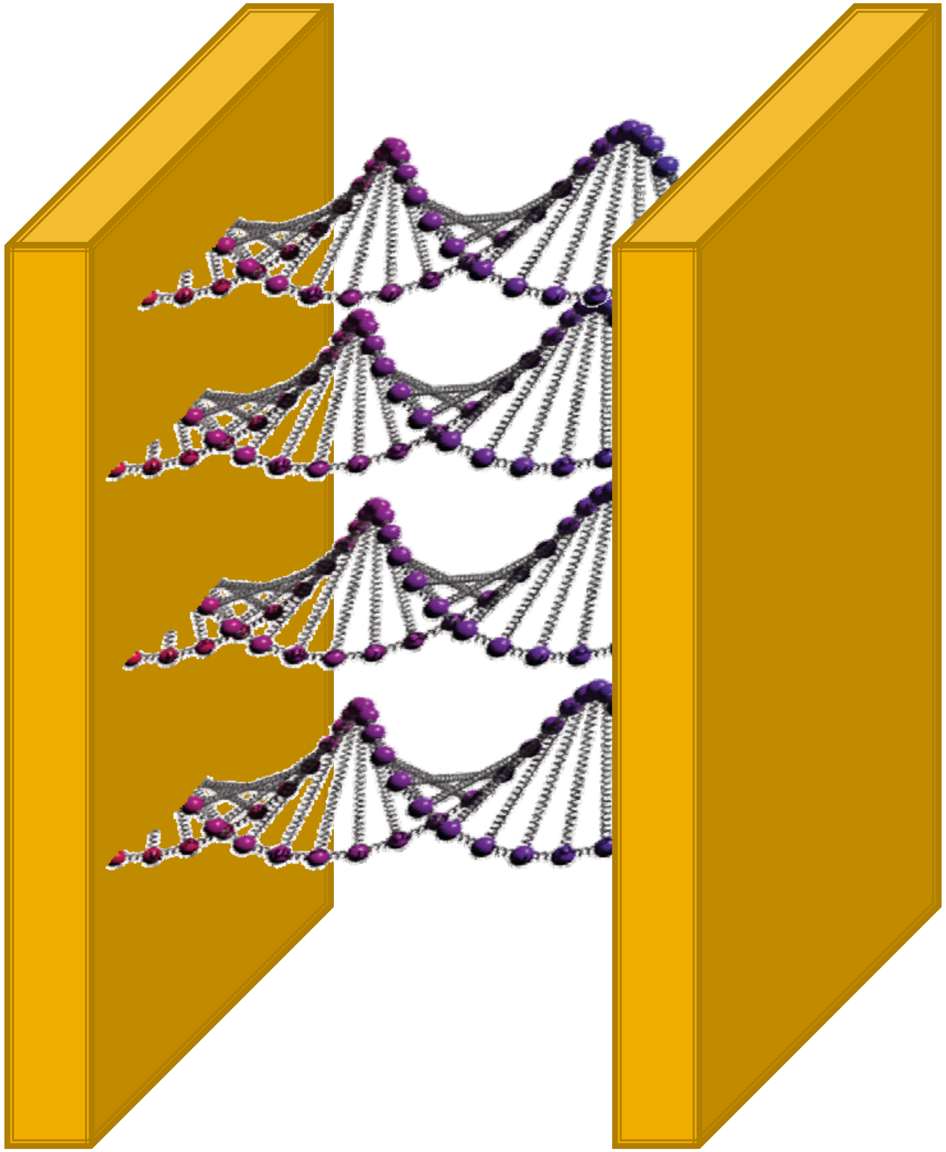




that each curled-up fragment can be considered as an individual thermal resistor R_{th}^*(ss-DNA) with a value of about 3.4×10^{12} °C/W. Interestingly enough, Velizhanin *et al.* predict for individual ds-DNA fragments a thermal conductivity of $\sigma_{th} = 1.8 \times 10^{-2}$ W/(°C·m) at 300 K.[21] Considering the 29-mer fragments as stiff rods with a length of 10 nm and a nominal radius of 1.2 nm, this conductivity translates to a resistance R_{th}^*(ds-DNA) = 1.2×10^{12} °C/W or roughly one-third of the value we derived experimentally for the disordered, single-stranded

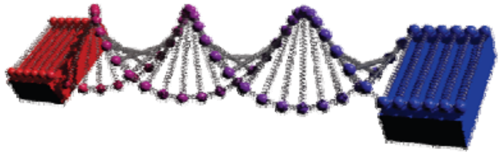
Van Grinsven *et al.*,
ACS Nano **6**, 2712 (**2012**)

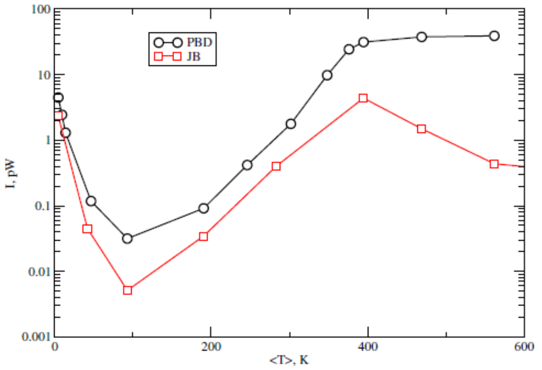
Possible thermal switch?



Open questions:

- How much of the $\kappa(T)$ is universal?
- Other systems with phase-transitions?
- From 1-coordinate to 2- coordinate models of DNA?





Thank you for listening ☺zzz

And thank the organizers again for a fantastic workshop!