



# Etude théorique de la translocation de biomolécules à travers un nanopore

Timothée Menais



28 février 2012

# Introduction

Translocation d'ADN à travers un nanopore

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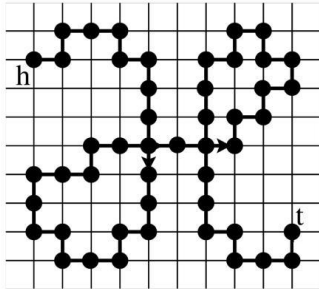
Translocation d'ADN à travers un nanopore  
Intérêts technologiques et fondamentaux

# Introduction

Translocation d'ADN à travers un nanopore  
Intérêts technologiques et fondamentaux  
Arrivée du graphène

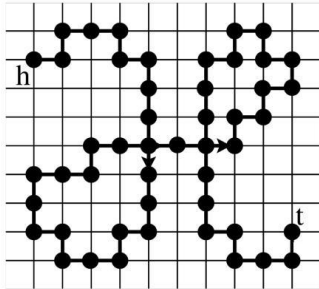
- 1 Outils analytiques
- 2 Dynamique moléculaire
- 3 Graphène

# Statique



[référence] H Vocks. Simulation of polymer translocation. Utrecht University, 2008.

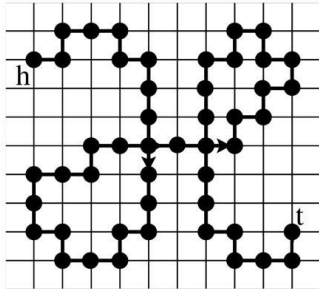
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$$Z_{ideal} = z^N \rightarrow Z_{nonideal} = \tilde{z}^N N^{\gamma-1}$$

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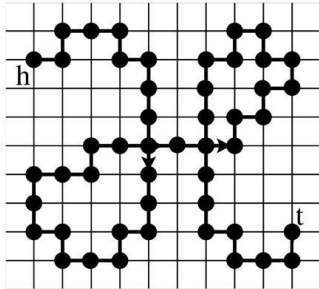
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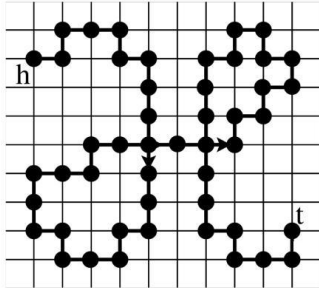
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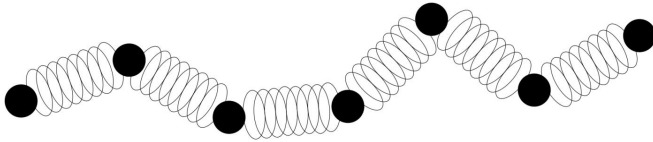
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$$F(r) = F(0) + \frac{3K_B T r^2}{2R_0^2} \text{ de type ressort}$$

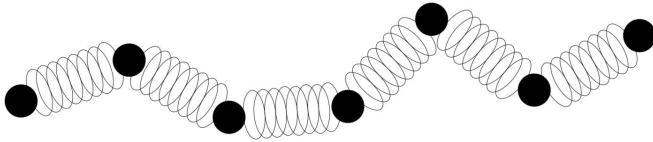
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# Modèle de Rouse



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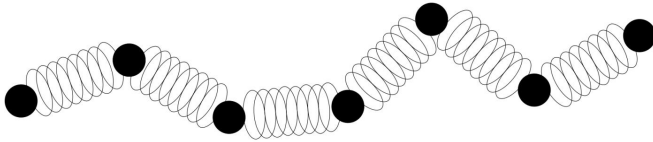
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$$\frac{d\mathbf{r}_n}{dt} = -\frac{1}{\epsilon} \frac{\partial F_{tot}}{\partial \mathbf{r}_n} + \mathbf{g}_n$$

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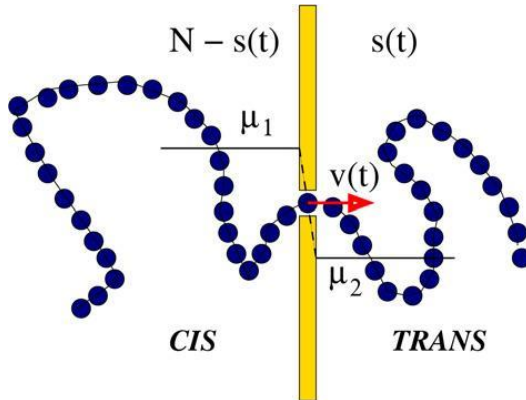


$$\frac{d\mathbf{r}_n}{dt} = -\frac{1}{\epsilon} \frac{\partial F_{tot}}{\partial \mathbf{r}_n} + \mathbf{g}_n$$

$$\langle (\mathbf{r}_{CM}(t) - \mathbf{r}_{CM}(0))^2 \rangle = \frac{6K_B T}{N\epsilon} t = 6D_R t$$

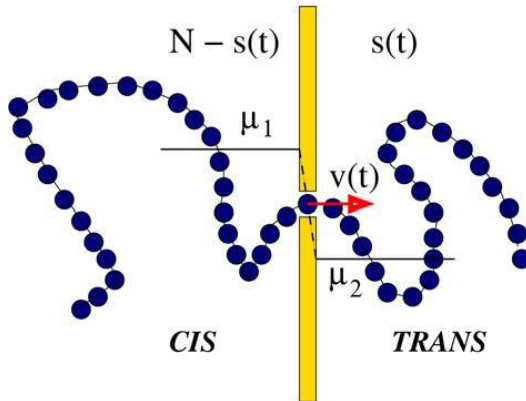
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# Translocation



[référence] A Milchev. Single-polymer dynamics under constraints : scaling theory and computer experiment. J Phys Condens Matter 23(10) :103101 (2011).

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$$\tau = N^\alpha f^{-\delta}$$

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$$F(N, n) = K_B T [(1 - \gamma_1) \ln[n(N - n)] - N \ln(\tilde{z})]$$

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$\tau$  est proportionnel à  $\frac{R_0^2}{D} \sim N^{1+2\nu}$

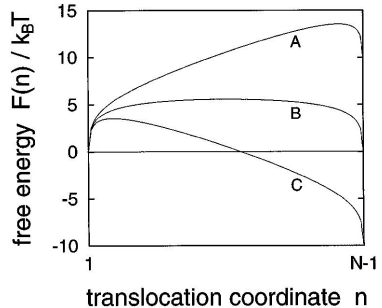
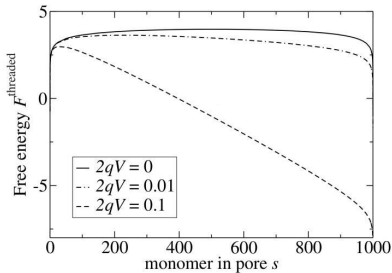
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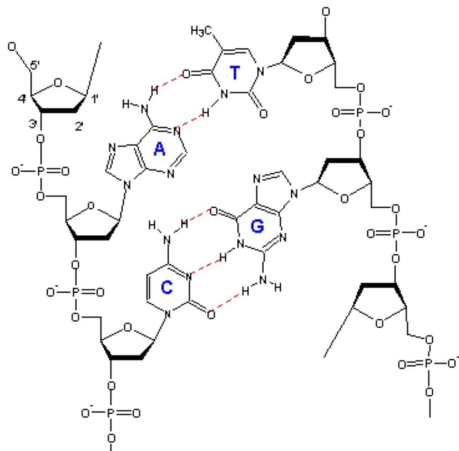
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# Nature de l'ADN



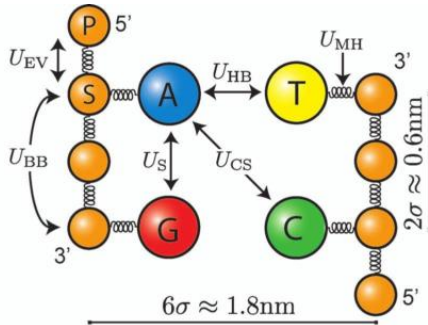
Structure

Liaisons covalentes

Liaisons hydrogènes

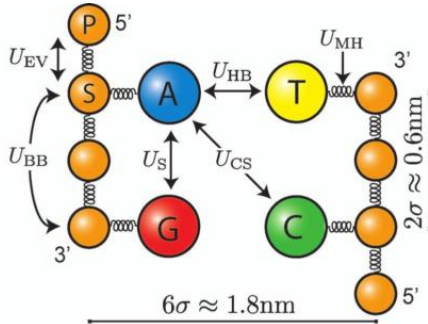
Interactions  
orbitales

# Modélisation



[référence] M. C. Linak, R. Tournier, and K. D. Dorfman. Moving beyond watson-crick models of coarse grained dna dynamics . *The Journal of Chemical Physics*, vol. 135, no. 20, p. 205102, 2011.

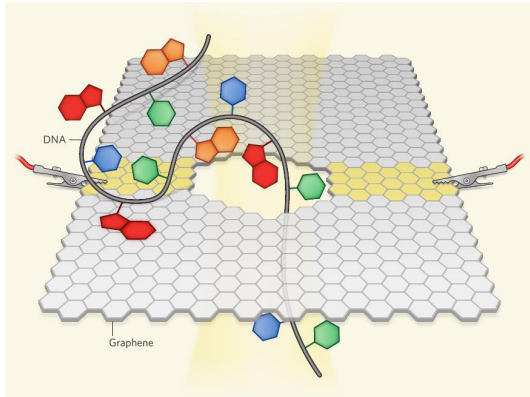
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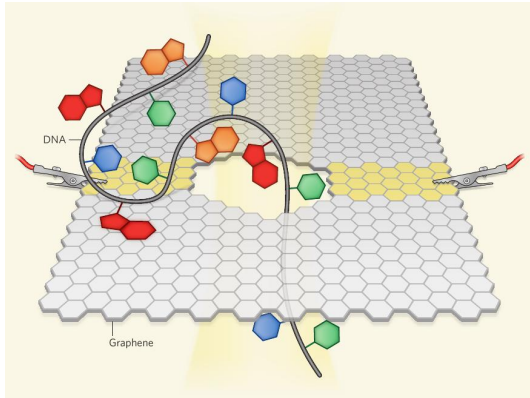
# Graphène



anciens pores rigides :  
biologiques et artificiels

[référence] H. Bayley. Nanotechnology : Holes with an edge . NATURE, vol. 467, p. 542, SEP 2010.

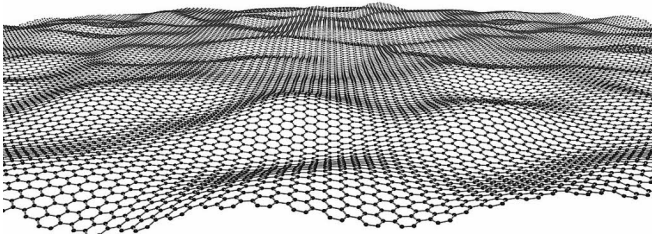
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# Graphène





# Conclusion

Utilisation d'outils analytiques et numériques

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Modélisation du graphène

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Utilisation d'outils analytiques et numériques

Modélisation du graphène

Temps de translocation, flexibilité et séquençage.

# Conclusion

Merci de votre attention.

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Des questions ?