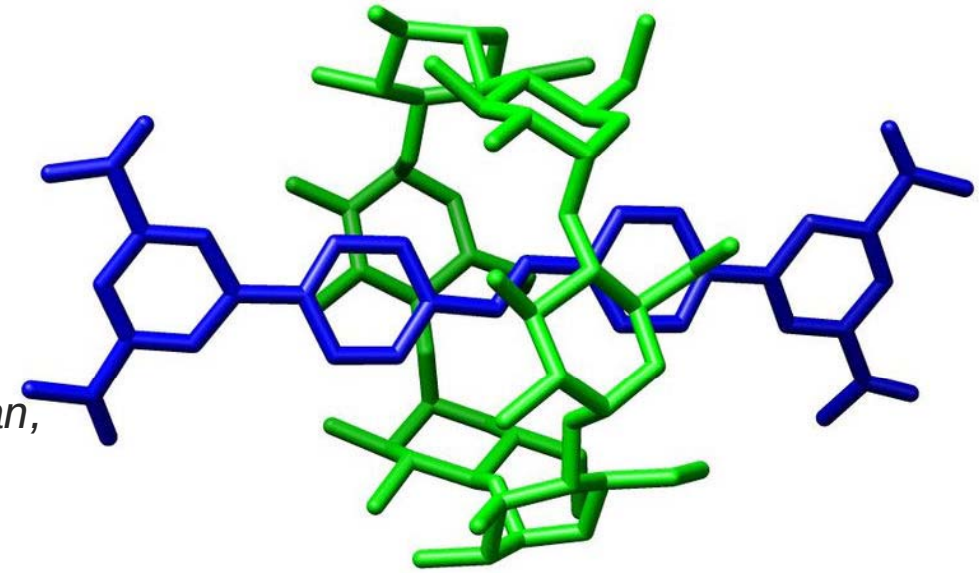
Study of Artificial Molecular Engines Action Through COMSOL Multiphysics Program

Lorenzo Moro

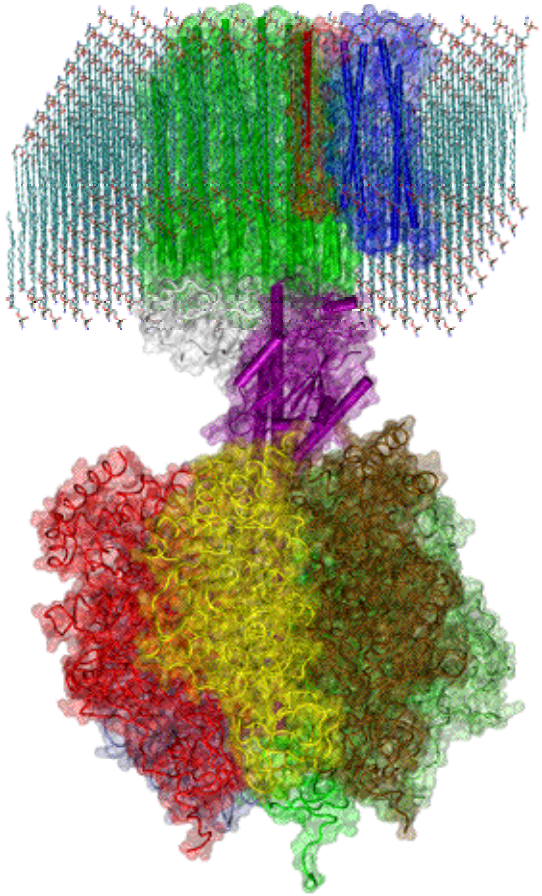
Francesca Lugli

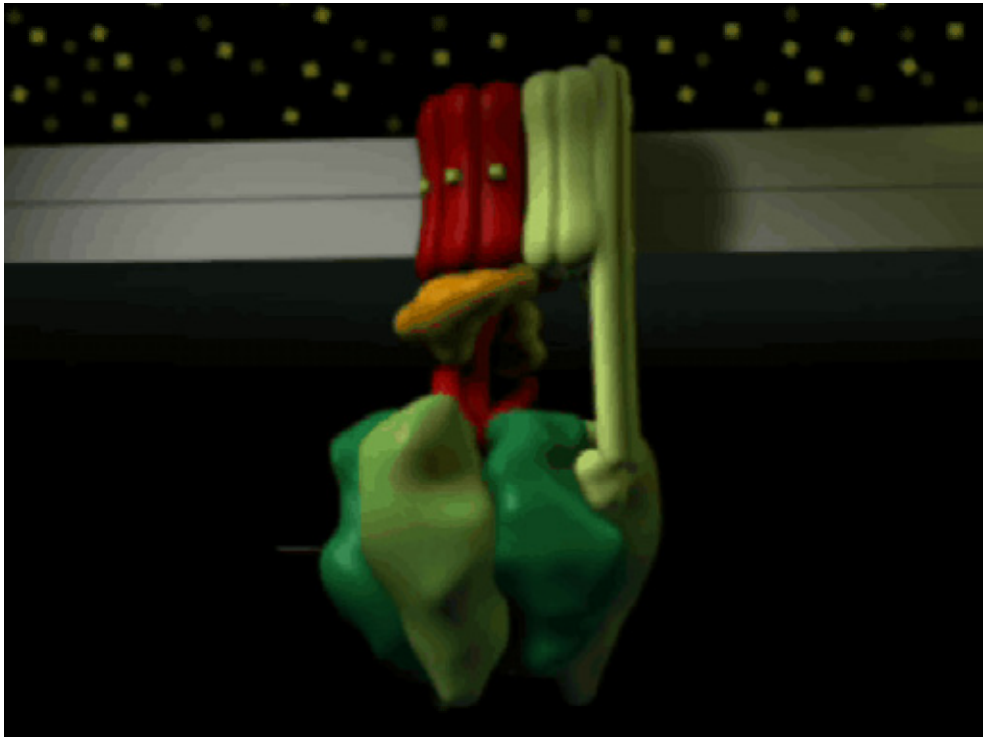
Francesco Zerbetto

Dipartimento di Chimica G.Ciamician,
Università di Bologna



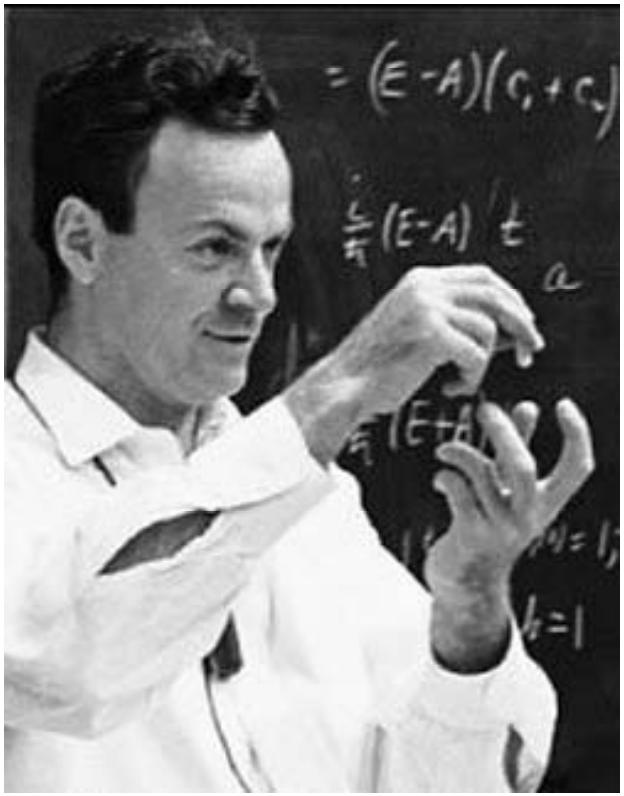
Molecular Motors in Nature: the ATPasi





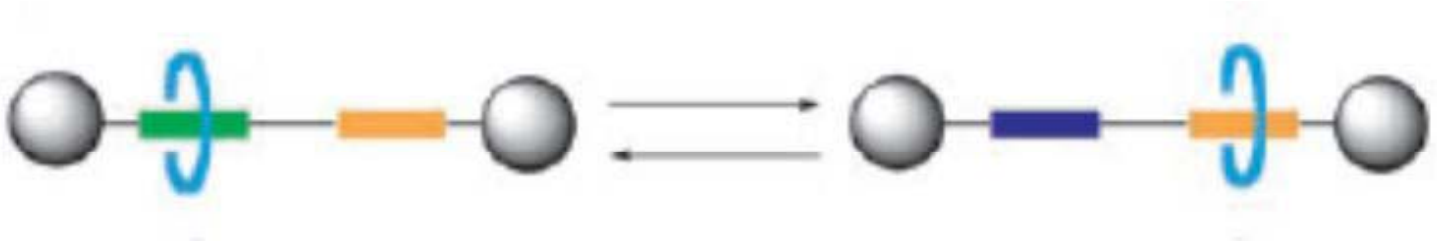
Artificial Molecular Motors

The idea to construct artificial molecular motos capable to do useful work was first advanced by Richard P. Feynman

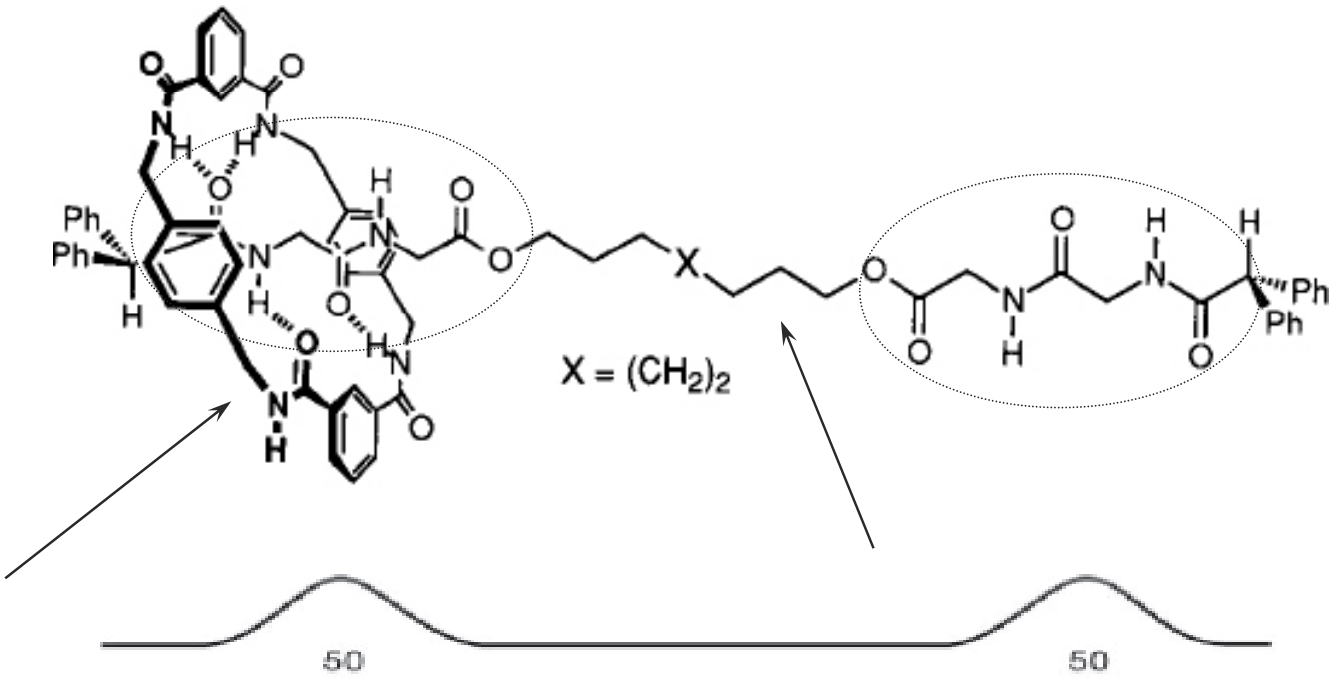


Artificial Molecular Motors

In the last years they have been succesfully developed; they can be of a various type

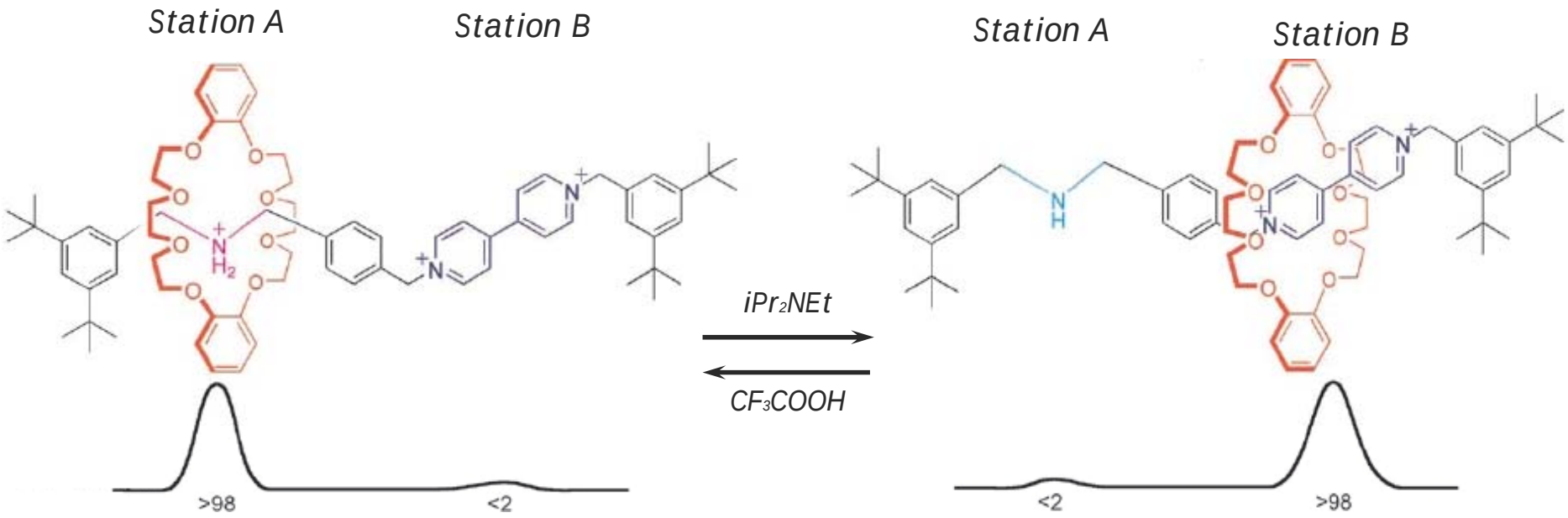


The Rotaxanes



A two stations switchable rotaxane

Switchable Rotaxanes



Is possible to control the position of the ring

Rationale of the Work

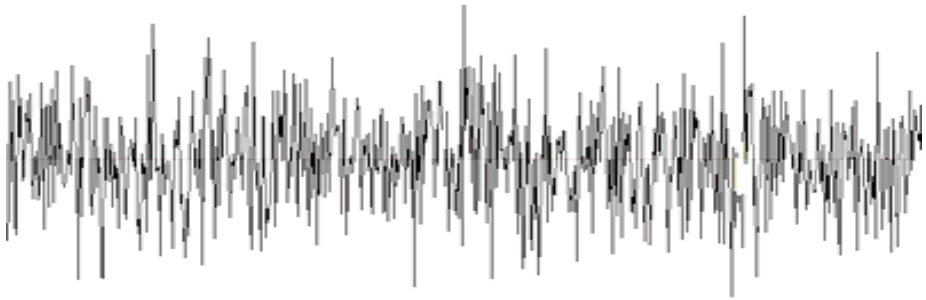
We want to quantify some mechanical parameters;

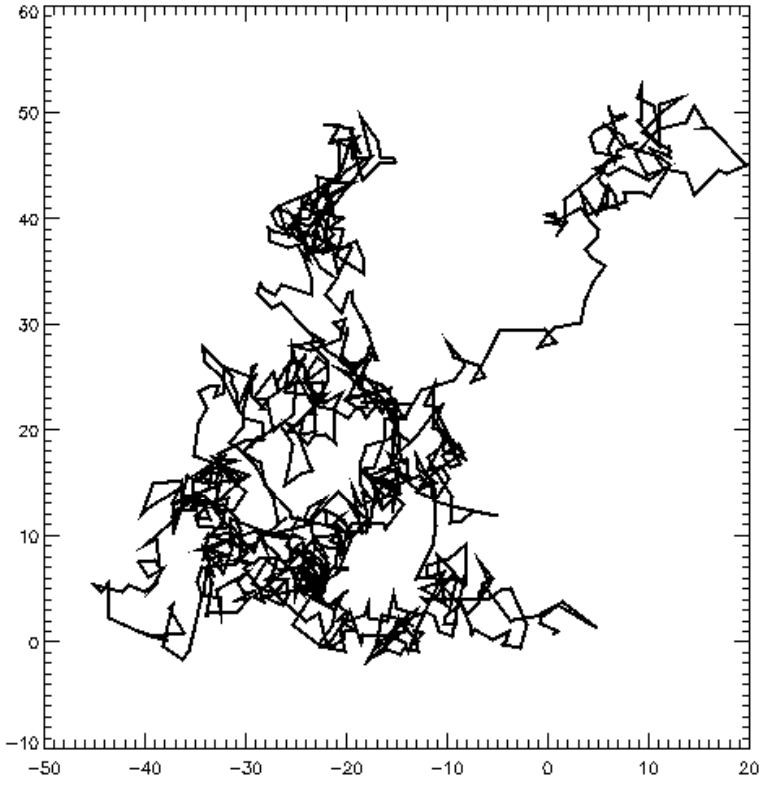
The distribution probability evolution in time is needed

Brownian Motion and Langevin Equations

$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx(t)}{dt} + F(t)$$

$F(t)$ describes the thermal fluctuations, it is called white noise





The Fokker-Planck Equation

From the Langevin approach is possible to find an equation of motion for the distribution probability. This leads to the 1-D Fokker-Planck equation:

$$\frac{\partial W(x,t)}{\partial t} = \left[\frac{\partial}{\partial x} U'(x) + D \frac{\partial^2}{\partial x^2} \right] W(x,t)$$

$$\frac{\partial W(x,t)}{\partial t} = L_{FP} W(x,t) \qquad D = k_B T (m\gamma)^{-1}$$

The Fokker-Planck Equation. Methods of solution

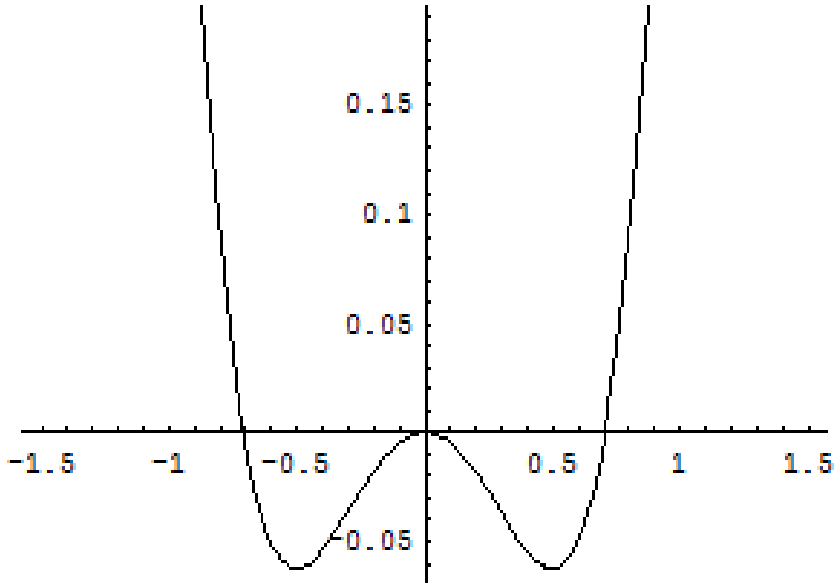
Stationary solutions → easily obtainable

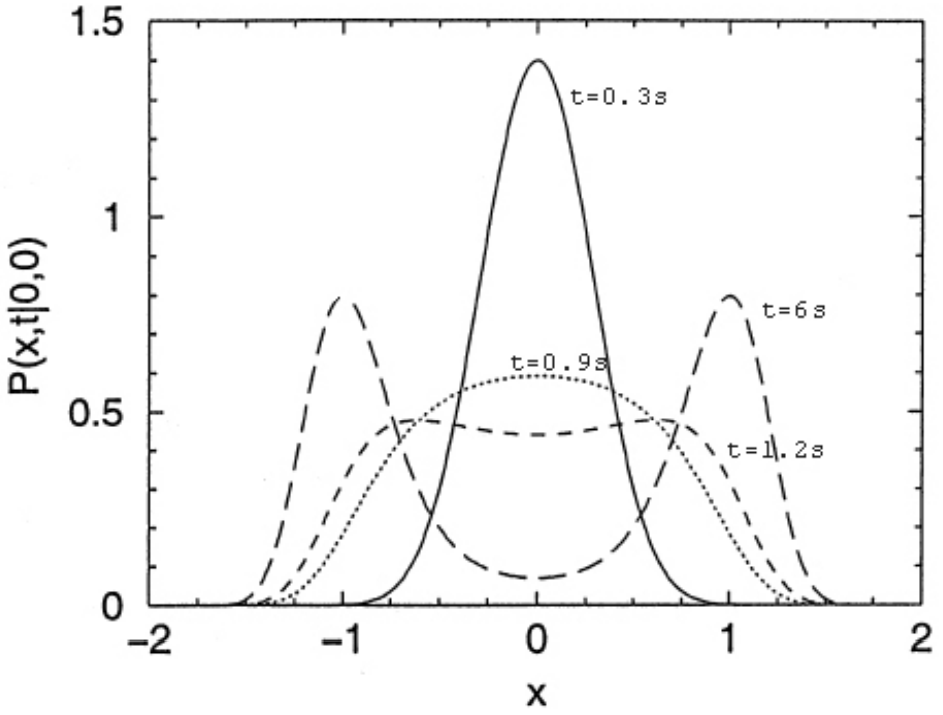
Nonstationary solutions → obtainable only in a few cases

$$\frac{\partial W(x,t)}{\partial t} = L_{FP} W(x,t) \longrightarrow L\Psi_n = -\lambda_n \Psi_n$$

$$L = D\frac{\partial^2}{\partial x^2} - V(x) \qquad V(x) = \frac{1}{4}\left[\frac{dU(x)}{dx}\right]^2 / D - \frac{1}{2}\left[\frac{d^2U(x)}{dx^2}\right]$$

Analitical solution for a simple bistable potential

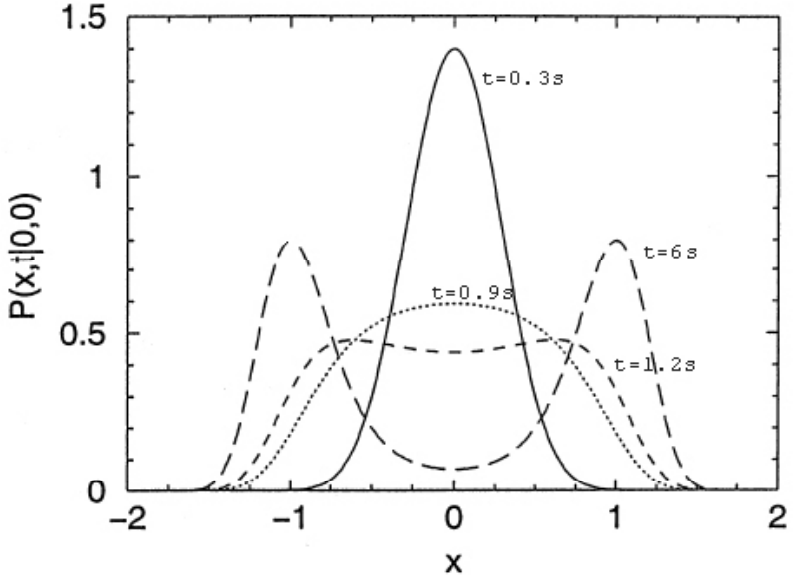


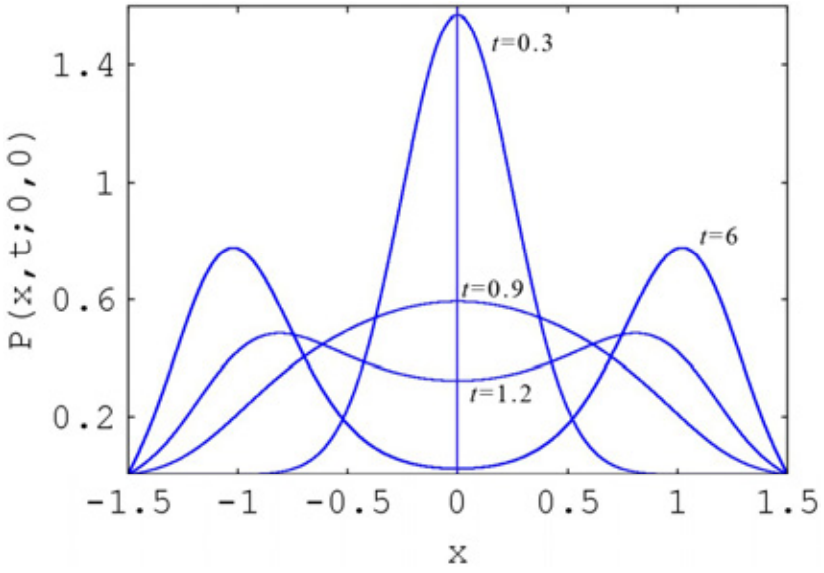


Ref. Phis.A 277 (2000) 335-348

Use of COMSOL

The first target is to find the match between the analytical solution and the computational one for the general Fokker-Planck equation



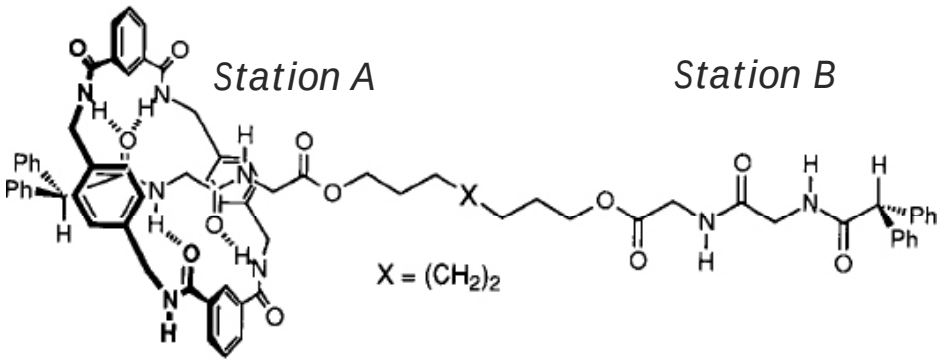


The Smoluchowski equation

$$\gamma v >> ma$$

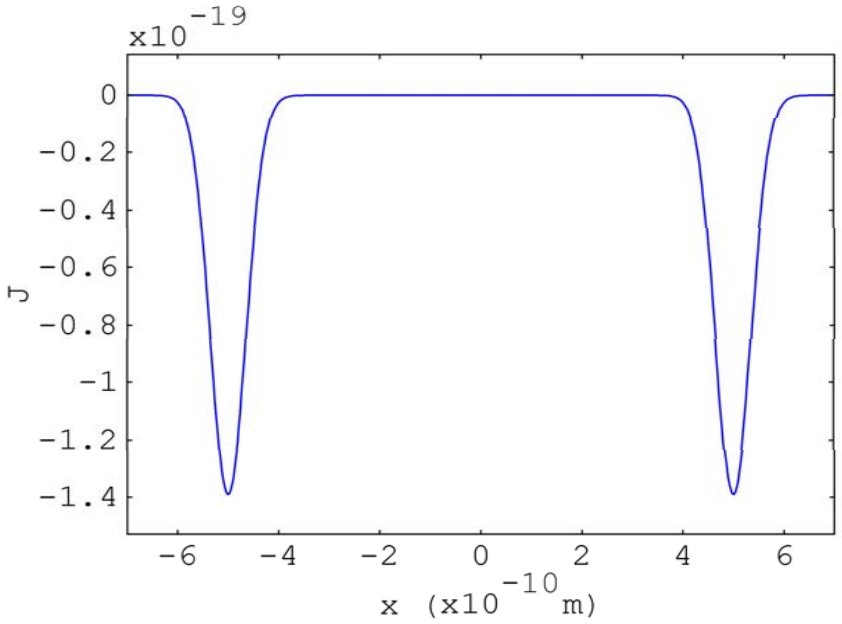
$$\frac{\partial W(x,t)}{\partial t} = \frac{1}{m\gamma}\left[-\frac{\partial}{\partial x}F(x) + k_B T \frac{\partial^2}{\partial x^2}\right] W(x,t)$$

Use of COMSOL with real molecules: Modeling the potential



U=-14 kcal/mol→1.389540028·10^{-19} J

Distance between the wells = 10Å



Use of COMSOL with real molecules: The Diffusion Coefficient

$$D = k_B T (m\gamma)^{-1}$$

Molecular Weight of the ring:533 g/mol

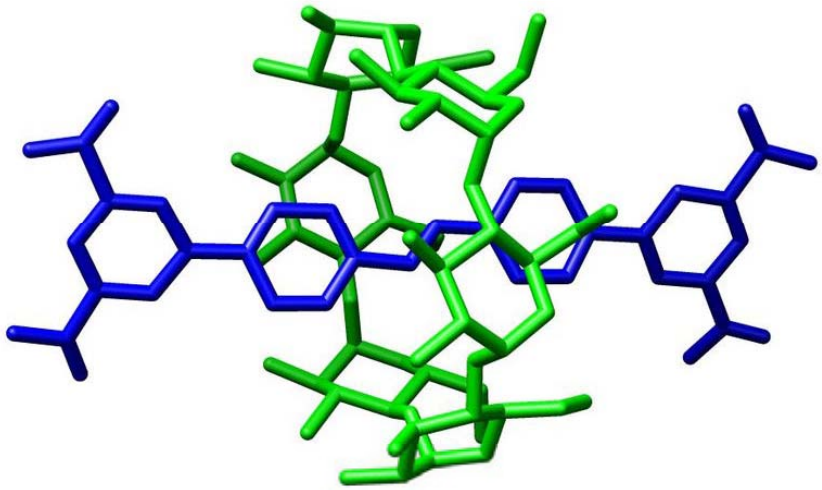
This rotaxane has best performances in MeOH and DMF which have different viscosity → different γ → different D

D_{MeOH}=3.64·10^{-10} m^2/s @ 298K

D_{DMF} =2.425·10^{-10} m^2/s @ 298K

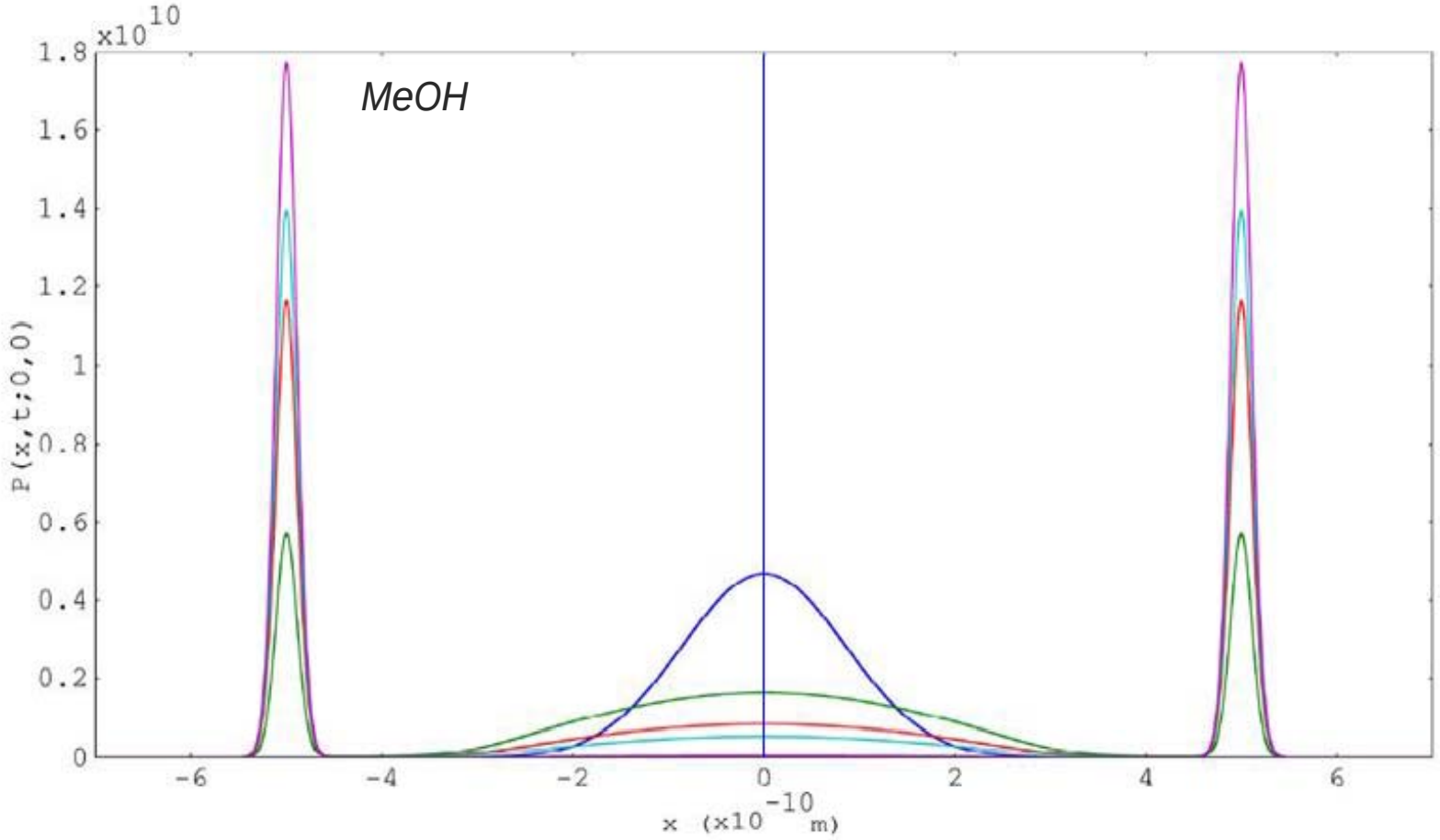
Use of COMSOL with real molecules: The Diffusion Coefficient

Before solving the system, a last consideration about D

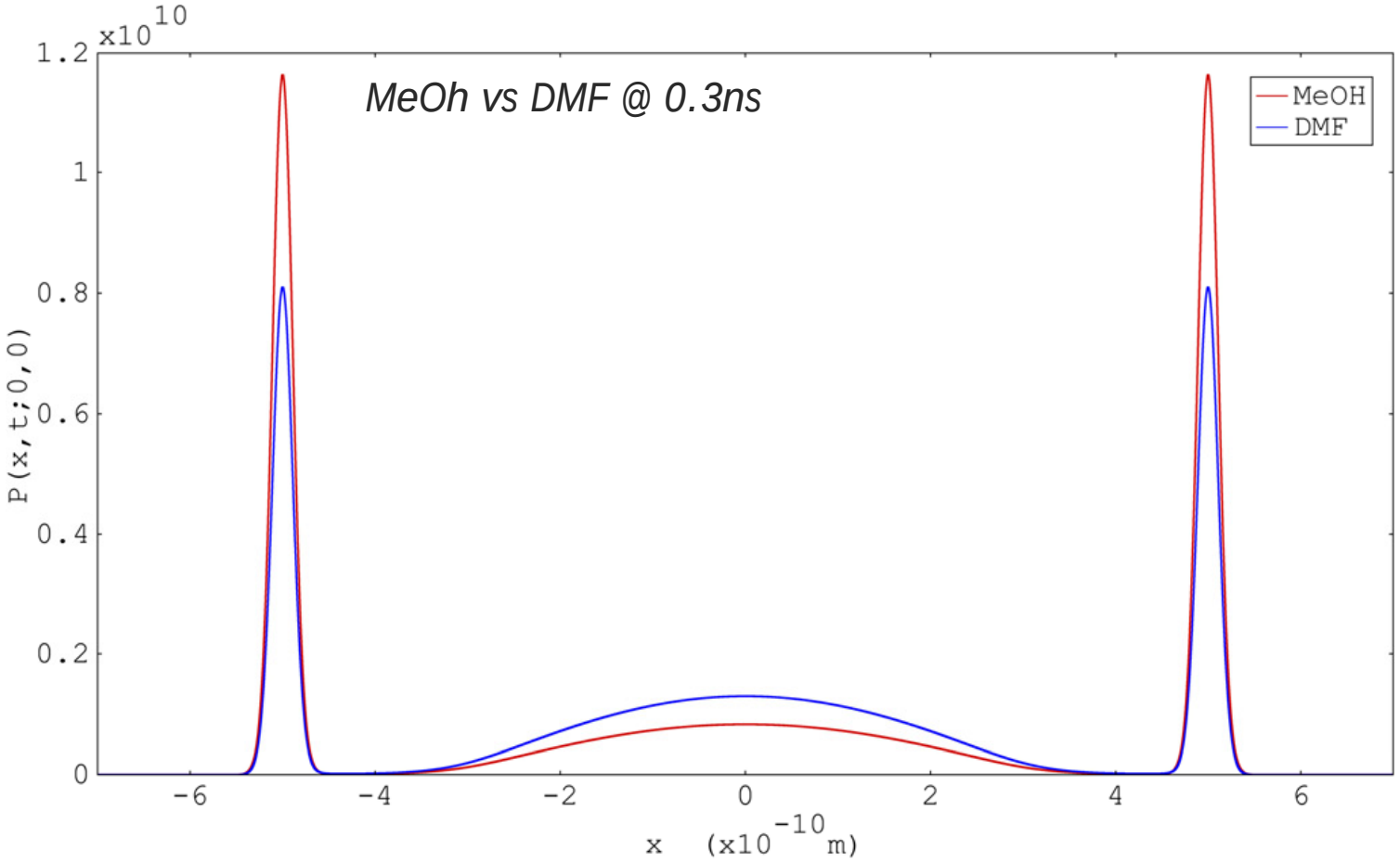


$D_{eff}=D/2$

Use of COMSOL with real molecules

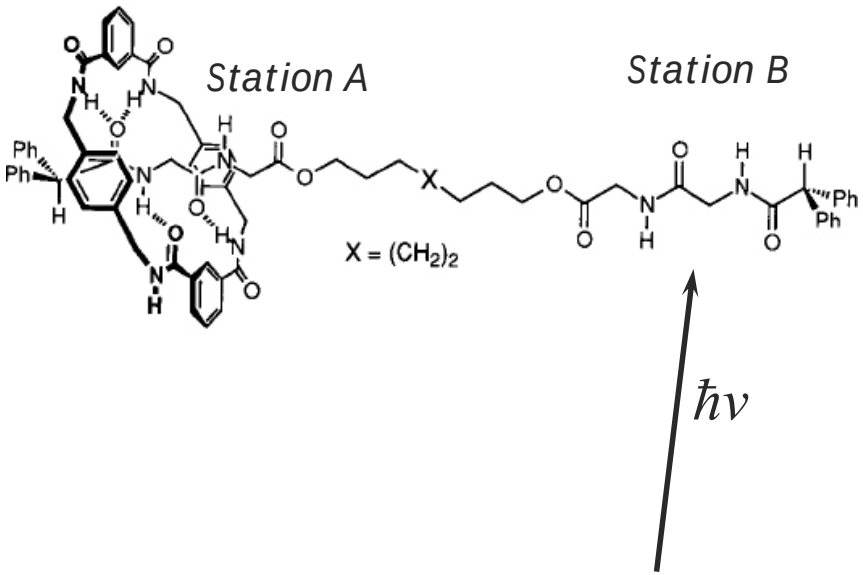


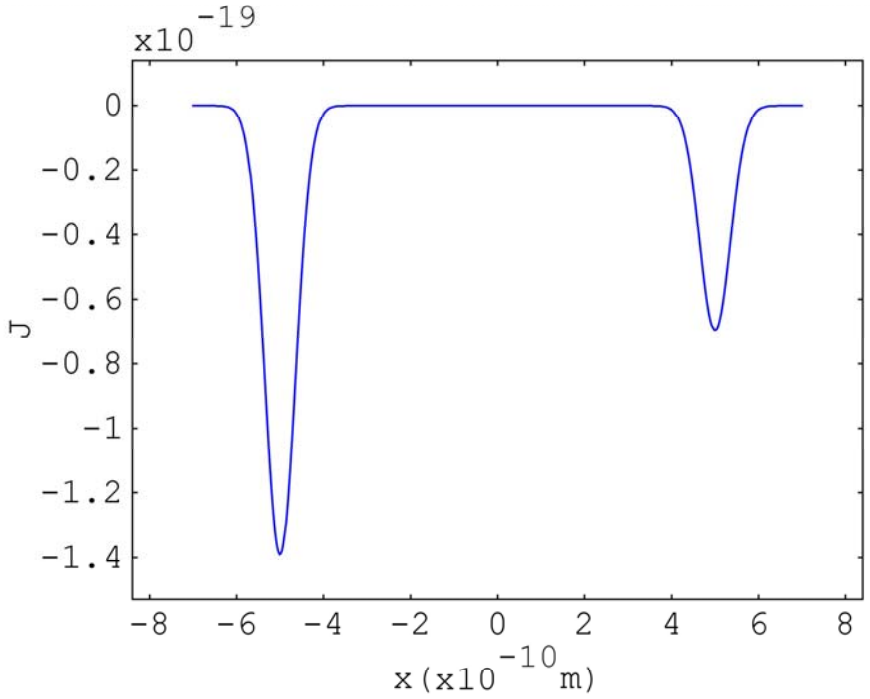
Use of COMSOL with real molecules



Use of COMSOL with real molecules

Making the ring where I want





Use of COMSOL with real molecules

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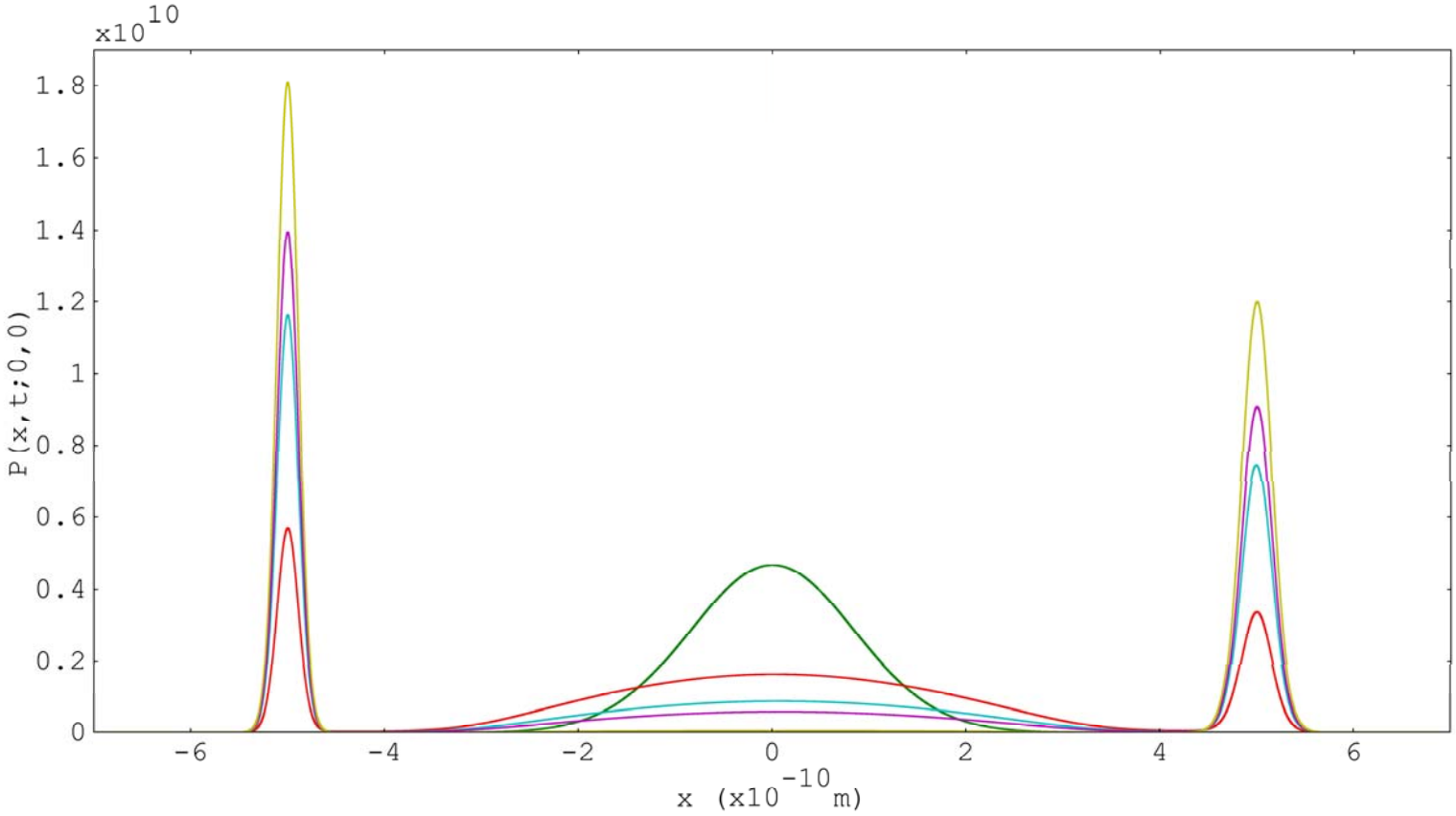

Future perspective

Calculation of Realistic Diffusion coefficients from Molecular Dynamics simulations.

Determination of the Useful system properties (Force and Entropy) from the solutions of the Fokker-Planck Equation

Thanks for the attention