



# "Soft-Matter Seminar"

**Maria Fyta**

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**Title:**

**Visualizing DNA: evidence from multiscale computer simulations**

**Abstract:**

Biophysical systems exhibit high complexity and diversity and need to be handled using different levels of sophistication at several length and time scales. These systems are studied by bridging the scales between the atomistic and the macroscopic through two different multiscale methodologies:

(a) Langevin Molecular-Dynamics techniques are concurrently coupled with a mesoscopic Lattice-Boltzmann method for the solvent dynamics to model biopolymer translocation through nanopores. Extensive simulations over various biopolymer conformations and lengths have been carried out, which probe the statistical nature of the process. The results overall agree well with recent experimental observations.

(b) Starting from accurate density-functional-theory simulations, a coarse-grained potential for DNA nucleotides is constructed and the electronic behavior of DNA bases and base-pairs is calculated. These calculations set the ground for a scheme that sequentially uses a semi-empirical quantum mechanical and an effective tight-binding model to study electron hopping and localization in stretched DNA.

**Mittwoch, den 2.4. 2008**

**13:00 Uhr**

**Raum PH 3344**

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