Design of nanomechanical sensors based on carbon nanoribbons and nanotubes in a distributed computing system

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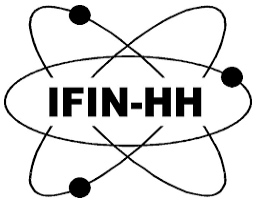
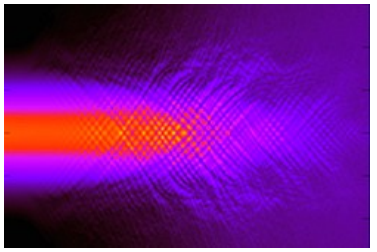


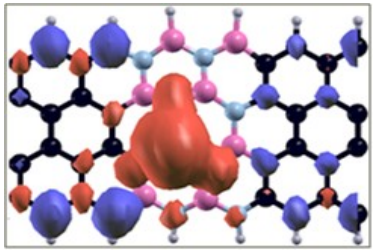
The 7th International Conference "Distributed Computing and Grid-technologies in Science and Education" (GRID 2016)

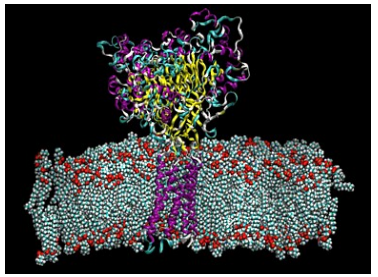
Presentation outline:

- Research strategy and computing infrastructure
- *Ab initio* simulation of nanostructures – SIESTA software package
- Density Functional Theory – SIESTA implementation
- Numerical tricks for simulation speedup
- Parallel SIESTA
- Nanomechanical resonators based on carbon nanoribbons and nanotubes
- Conclusions

Research strategy and computing infrastructure







The main strategic directions for R&D of the CPIT Department are:

- Numerical investigation of mesoscopic quantum systems
- High-performance computing for applications in nuclear and condensed matter physics
- *Study of physical properties of nanostructures through ab initio computing methods*
- Computational modeling and simulation of condensed systems with many interacting particles
- Modeling and simulations in biophysics

Computing infrastructure:

- IBM BladeCentre H
  Infiniband Voltaire 4X (40Gbps)
- 10 nodes LS22 + 16 nodes QS22
  - 80 cores AMD Opteron, 80GB RAM
  - 32 PowerXCell 8i, 512GB
- 56 nodes HS22: 2x Intel Xeon X5650 @ 2.67GHz (6 Core)
  - 672 cores,
  - 2412 GB RAM @ 1333 MHz
  - 500GB SATA3 HDD per node
- 7 nodes HS23: 2x Intel Xeon E5-2670 @2.60GHz (8 core)
  - 112 cores
  - 420 GB RAM @ 1600MHz
  - 500GB SAS HDD per node
  - 4x NVIDIA Tesla M2090 GPU
    Graphics clock: 650 MHz
    Processor clock: 1300 MHz
    Memory size: 6GB GDDR5
    CUDA cores: 512
- Storage 35TB Raid6 w GbE
  Storage 14TB Raid6 w IB
  Storage 66TB Raid6 w IB

Ab initio simulation of nanostructures – SIESTA software package

- **SIESTA** - Spanish Initiative for Electronic Simulations with Thousands of Atoms

  "The SIESTA method for ab initio order-N materials simulation" José M Soler, Emilio Artacho, Julian D Gale, Alberto García, Javier Junquera, Pablo Ordejón and Daniel Sánchez-Portal
  J. Phys.: Condens. Matter 14 2745 (2002)

- SIESTA 4.0 (GPL license) – departments.icmab.es/leem/siesta/

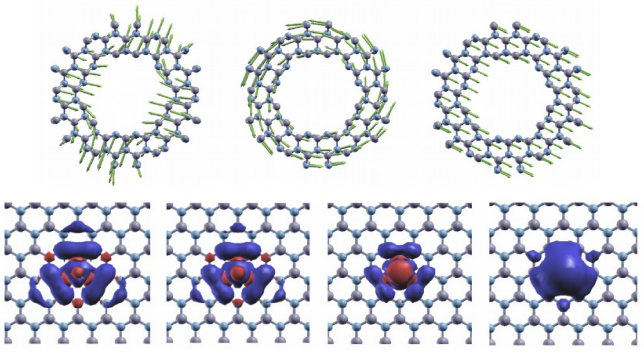
- Most important feature of SIESTA: **linear scaling**, while usual DFT methods scale as $\mathbf{N^3}$!

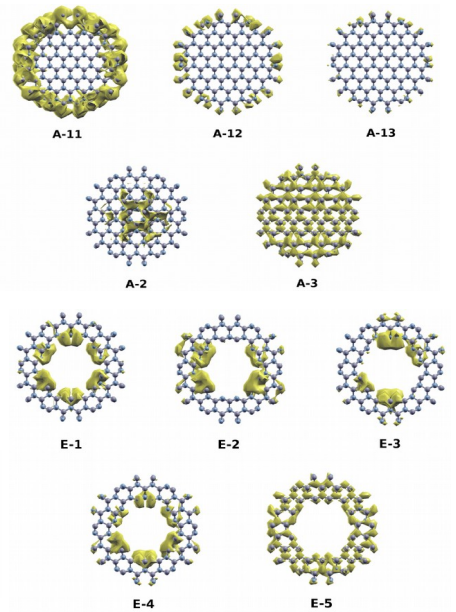
What can you compute with it ?

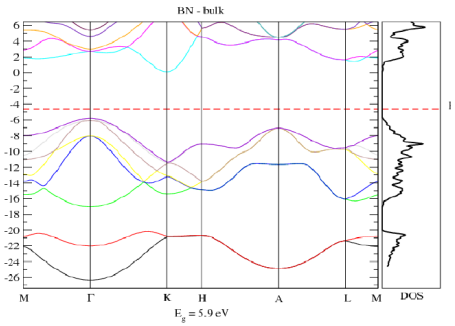
- Electronic band structure
- Electron density
- Total and partial density of states
- Electric dipole moment
- Mulliken population
- Spin polarized calculations
- Atomic forces
- Structural relaxation
- Stress tensor
- Moleculat dynamics
- Phonon spectra

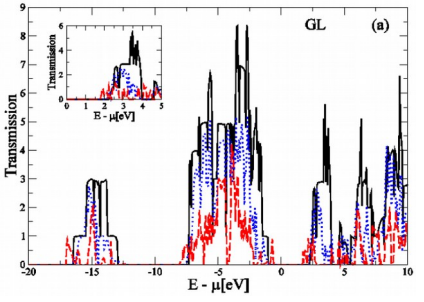
What else can it do ?

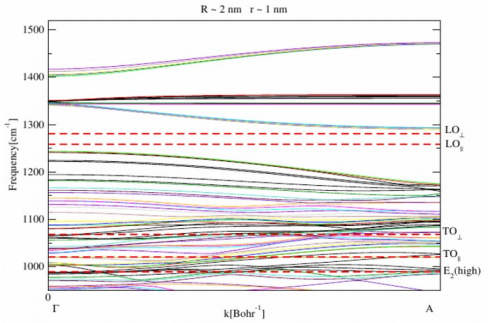
Ballistic electronic transport with **TRANSIESTA**
"Density-functional method for nonequilibrium electron transport" Mads Brandbyge, Jose-Luis Mozos, Pablo Ordejon, JeremyTaylor, and Kurt Stokbro
Phys. Rev. B 65 165401 (2002)

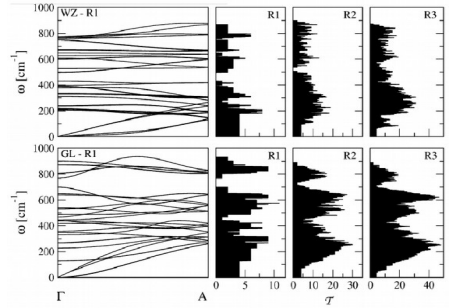












Density Functional Theory – SIESTA implementation

- **Traditional approach:** find approximate solutions for the Schrödinger equation

$$\left\{ -\frac{h^2}{2m}\sum_j \nabla_j^2 - \sum_{j,i}\frac{e_0^2 Z_i}{|r_j - R_i|} + \frac{1}{2}\sum_{j\neq i}\frac{e_0^2}{|r_j - r_i|} - E \right\} \psi(r_1, ..., r_N) = 0$$

Not trivial even for N=2 !

- **Density Functional Theory (DFT):** Hohenberg & Kohn & Sham

  Main ideas:

  - replace the N electron wavefunction with a density functional for non interacting electrons

  - include all multi-particle effects in a separate energy term known as the exchange correlation energy (E_{xc})

- P. Hohenberg and W. Kohn **Phys. Rev., 136 B864 (1964)**
- W. Kohn and L. J. Sham **Phys. Rev., 140 A1133 (1965)**

- **Kohn-Sham equations:**

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{KS}(\vec{r}) \right) \psi_i(\vec{r}) = E_i \psi_i(\vec{r}) \qquad E[\psi_i(\vec{r})] = T_e + U_{nn} + U_{ne} + U_{ee} + E_{xc}$$

Schrödinger-like equation for system of non-interacting particles that generates the **same electron density as the real system of interacting particles**.

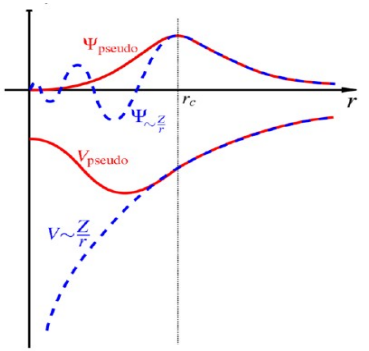
- *Solve the KS equations by minimizing the energy of the system – variational approach.*

Numerical tricks for simulation speedup

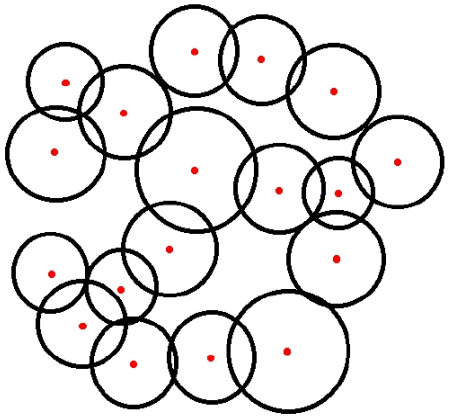
- Use **pseudopotentials**: replace core electrons and nuclear potential with an effective pseudo-potential.
- **Benefits of using pseudopotnetials:**

  - Get rid of core electrons (not chemically active)
  - Iron out strongly varying wavefunction (near core)

  → *Reduce the number of electrons and the basis set that will be required.*



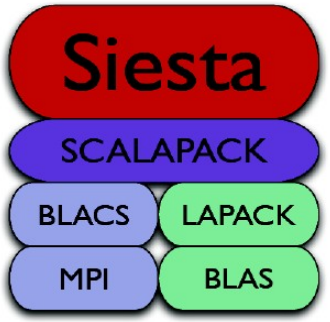
- Use soft pseudopotentials for **transferability** (compute once and use in any system)



- Numerical orbitals: SIESTA uses a **localized basis set** which leads to **sparse Hamiltonian and overlap matrices + empty space has almost no additional computational cost**
- **Periodic Born - von Karman boundary conditions:** easily solve infinite systems but can also treat non-periodic systems if the supercell is large enough
- **Monkhorst-Pack** scheme for Brillouin zone integration

SIESTA software stack:

- **MPI** communication layer
- **BLACS** basic linear algebra library with integrated MPI communication
- **SCALAPACK** linear algebra package: uses BLAS + LAPACK for serial operations and MPI+ BLACS for parallel operations



Parallel SIESTA

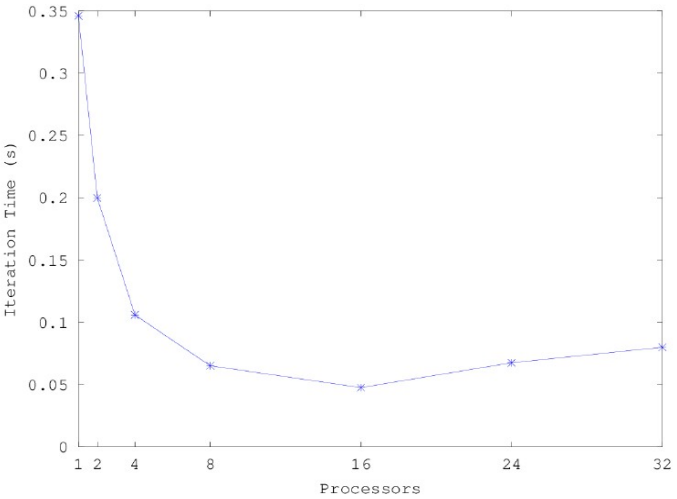
- **Main parallelization options:**

  - Parallel over K: solve problem for each separate reciprocal space point

  - Solve eigenvalue problem by parallel matrix diagonalization

  - Spatial decomposition based on atomic proximity

- **Difficult to test scaling because of a large variety of physical systems and numerical requirements**: 1D, 2D, 3D, periodic, non-periodic, number of atoms, different numerical accuracy required for different investigated parameters, etc.



Georg Huhs - “Parallelization issues” (handout)

Personal user-case results:

- Optimal configuration: **8 cores** (on same processor) per instance while running multiple independent instances

- Possible **speedup** from library and architecture optimization: over **2.7 times**

- **HPC scaling for DFT simulations:**

  - *“Performance Analysis of Electronic Structure Codes on HPC Systems: A Case Study of SIESTA”* F. Corsetti, **PLoS ONE 9 e95390 (2014)**

  - *“Linear-scaling density-functional theory with tens of thousands of atoms: Expanding the scope and scale of calculations with ONETEP”* N.D.M. Hine, P.D. Haynes, A.A. Mostofi, C.-K. Skylaris, M.C. Payne, **Comp. Phys. Comm. 180 1041–1053 (2009)**

Nanomechanical resonators based on carbon nanoribbons and nanotubes

- **Motivation:**

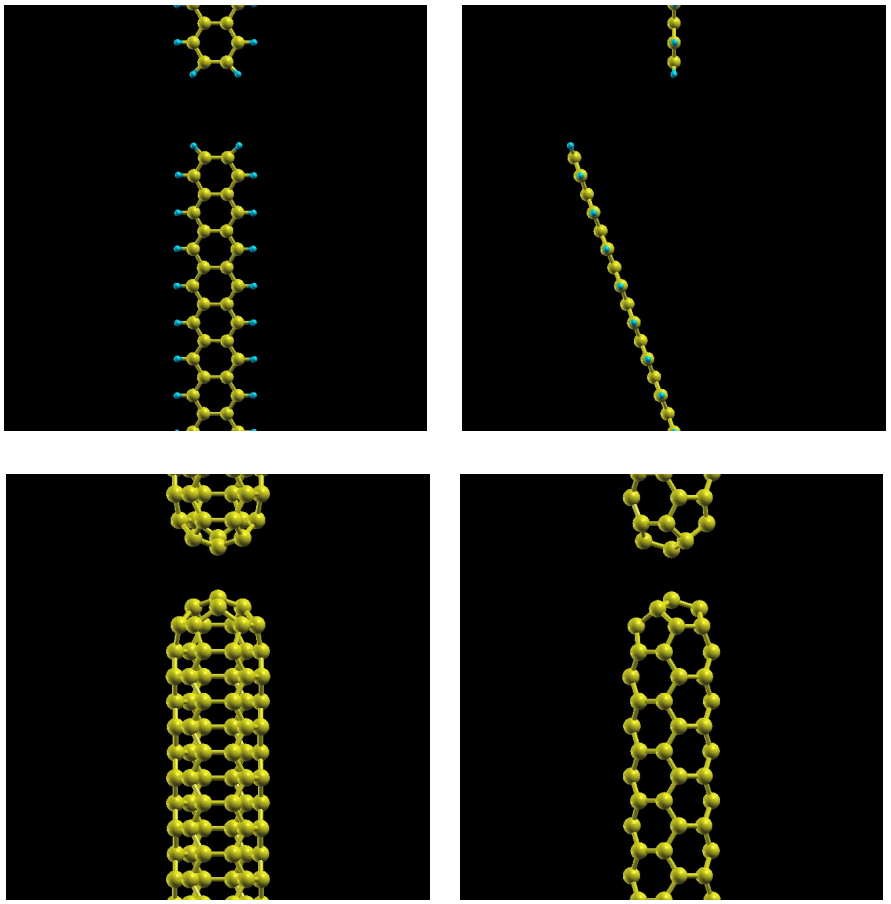
  - multiple possible practical uses such as: high-frequency oscillators or ultra-sensible acceleration detectors

- **Possible practical implementation:** measure transmission current between oscillator tip and contact to estimate position and frequency

- **Systems studied:**

  - monoatomic thickness nanoribbons of length 17.3 Å and 2.8 Å diameter made out of 32 C atoms and passivated with 18 H atoms

  - nanotubes of length 35.9 Å and 4.2 Å diameter made out of 92 C atoms with closed ends



- **Simulation parameters:**

  - basis type: double zeta polarized

  - local density approximation functional (LDA) + Ceperley Alder exchange correlation parametrization

  - 300 Ry mesh cut-off, 10^{-3} density matrix tolerance, 0.01 eV/Ang maximum force tolerance

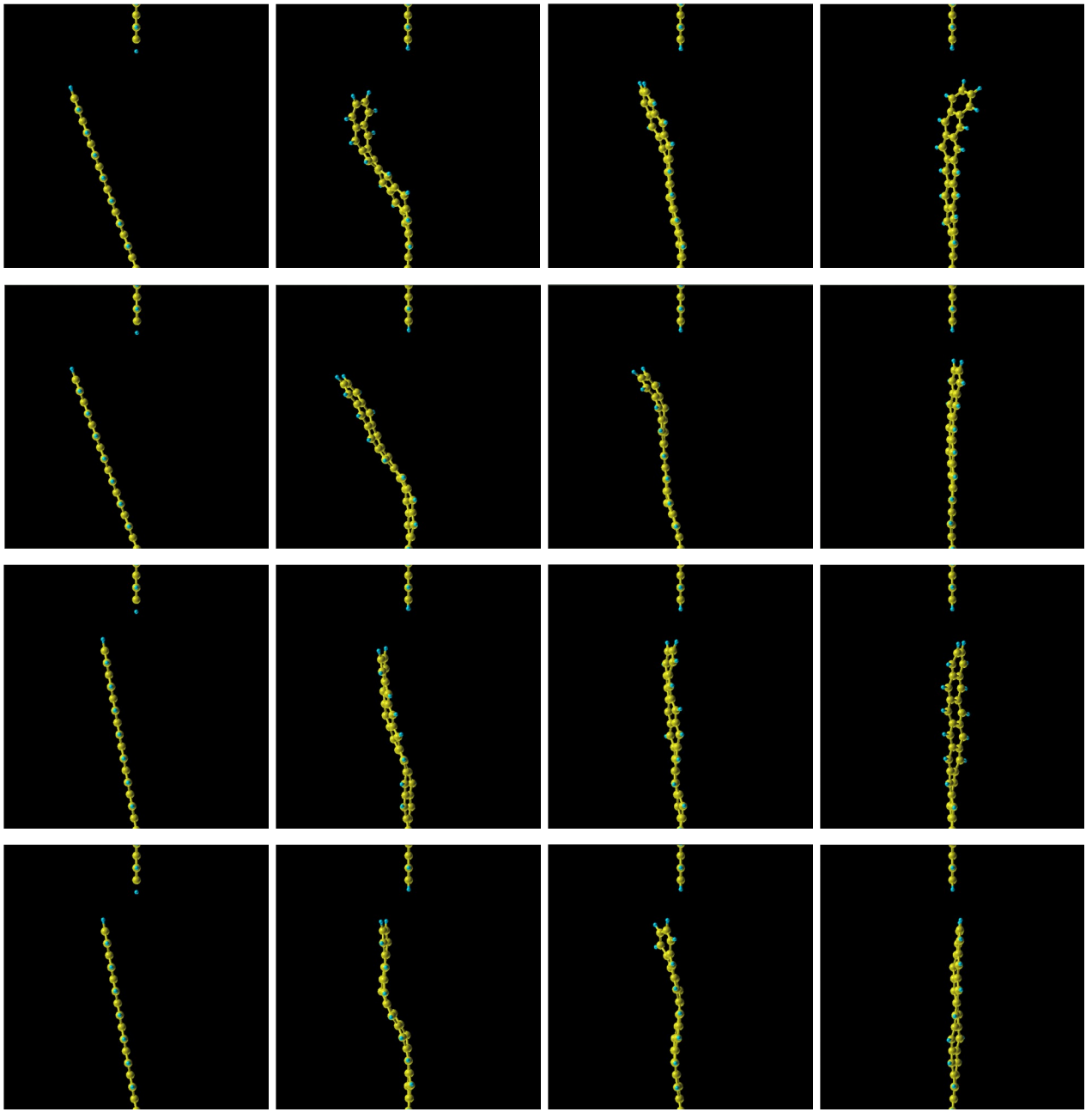
- **Goals:**

  - structural relaxation + molecular dynamics with thermostat at 300 and 150 K

  - transmission function over gap (between nanotube and contact) for different separations (TRANSIESTA - NEGF)

Nanomechanical resonators based on carbon nanoribbons and nanotubes

Time: 0 (fs) 1000 (fs) 2000 (fs) 3000 (fs)



Initial angle = 20°
T = 300 K

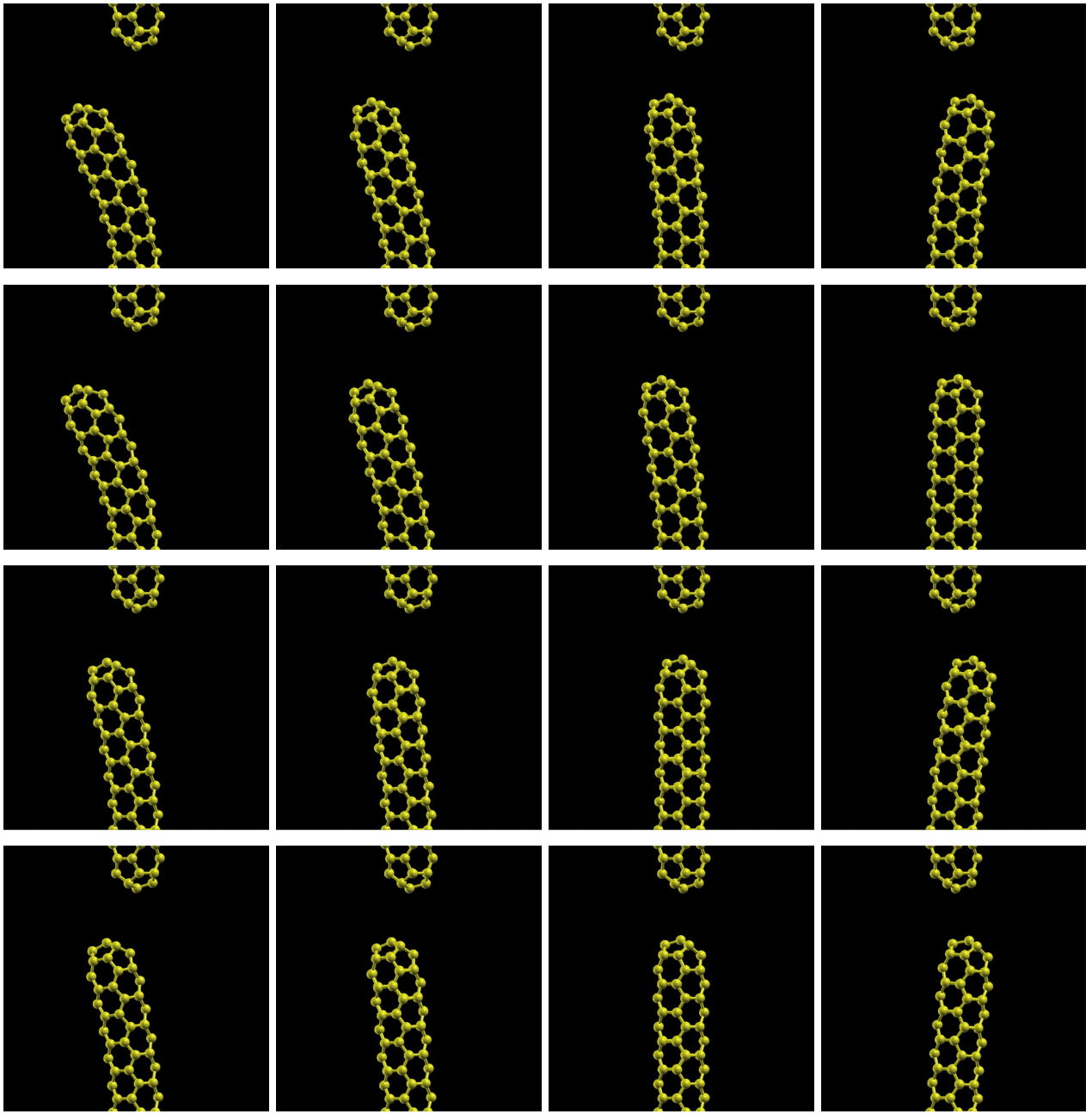
Initial angle = 20°
T = 150 K

Initial angle = 10°
T = 300 K

Initial angle = 10°
T = 150 K

Nanomechanical resonators based on carbon nanoribbons and nanotubes

Time: 0 (fs) 200 (fs) 400 (fs) 600 (fs)



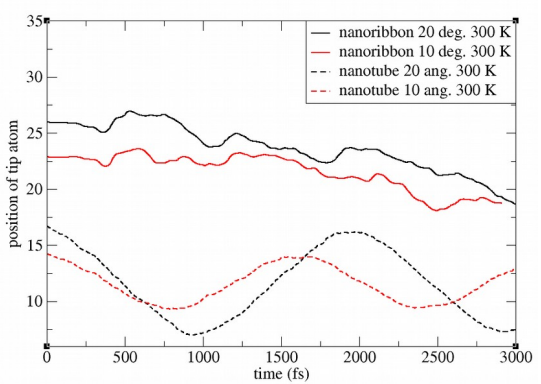
Initial angle = 20°
T = 300 K

Initial angle = 20°
T = 150 K

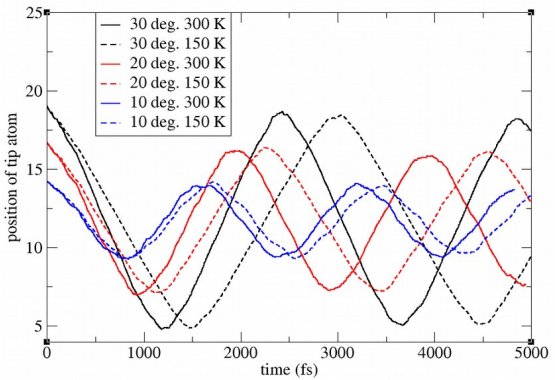
Initial angle = 10°
T = 300 K

Initial angle = 10°
T = 150 K

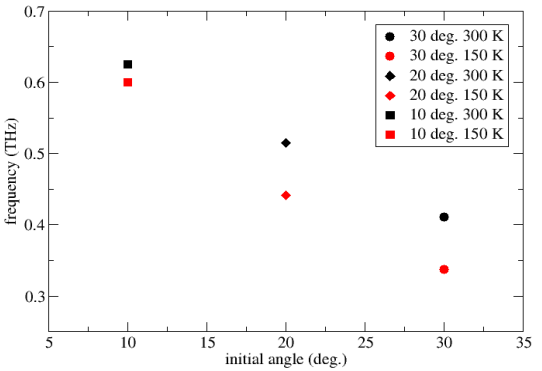
Nanomechanical resonators based on carbon nanoribbons and nanotubes



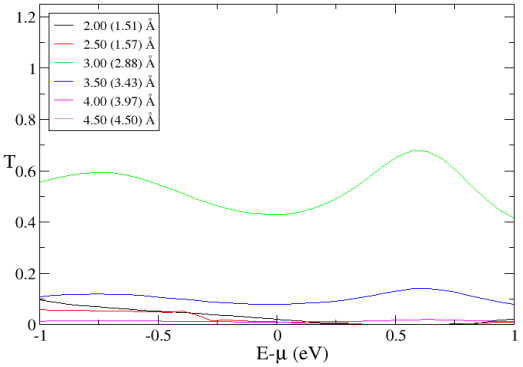
Position of tip atom in oscillation plane as a function of time for the first 3000 fs: *nanoribbon vs. nanotube*



Position of tip atom of *nanotubes* in oscillation plane as a function of time for the first 5000 fs



Resonant frequency of *nanotubes* as a function of the initial angle



Transmission from -1 to 1 eV as a function of *nanotube*-contact distance (initial and after relaxation)

Conclusions:

- Because of the reduced rigidity, the studied **nanoribbons have a much higher period of oscillation** and are **more susceptible to thermal noise** than the nanotubes. This makes **nanotubes better suited as nanomechanical resonators**.
- The **nanotubes show a non-linear behavior**, with a resonant frequency that depends on both the initial amplitude (angle) and also on temperature.
- The **nanotube-contact gap** has an **optimal value of ~3 Å**
- Small diameter nanotubes prove to be suitable candidates for **nano-resonators in the THz region**

Thank you for your attention !