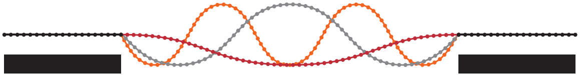
Nanomechanics of Graphene Membranes

vibrational modes on the nanoscale



Christoffer Vendelbo Sørensen   Frederik Grunnet Kristensen
Rasmus Kronborg Finnemann Wiuff
Supervisors: Mads Brandbyge   Tue Gunst

Technical University of Denmark

April 18, 2018

Outline

- Graphene: 2D Carbon lattice

Introduction

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- Prominent properties

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  "Visualizing the Motion of Graphene Nanodrums"
  Nano Letters **16**, 2768-2773 (2016)
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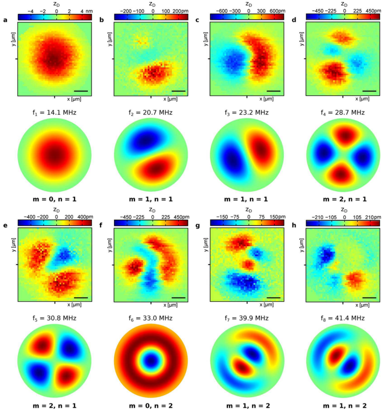

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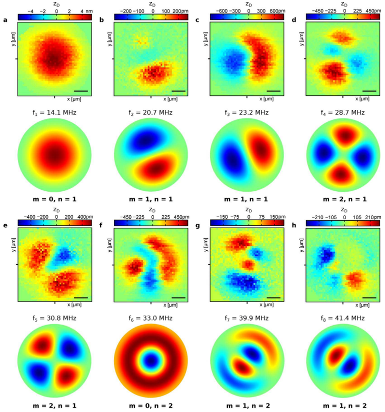

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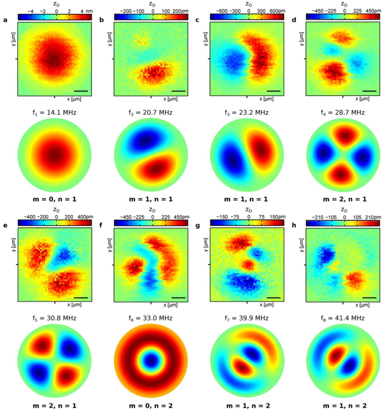
- Microdrums on the micron scale
- Nanomembranes on the nanometer scale

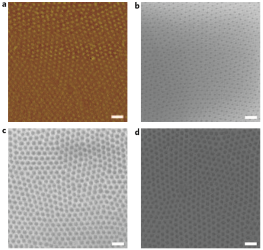


Introduction

Hypothesis:

Does drum modes exist in graphene supported by a nanomesh with nanometer sized holes?

Jingwei Bai, Xing Zhong, Shan Jiang, Yu Huang, and Xiangfeng Duan
"Graphene nanomesh"
Nature Nanotechnology **5**, 190-194 (2010)
arXiv:NIHMS150003



The Dynamical Matrix

- Matrix in Eigenvalue problem (below)

$$M\omega_{\mathbf{q}}^2 \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix}$$

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- Matrix in Eigenvalue problem (below)
- Elements in matrix are Fouriertransform of the spring constants between configuration atoms
- Essential for calculating vibrational modes

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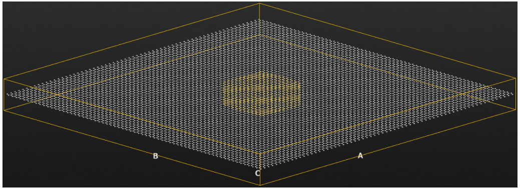
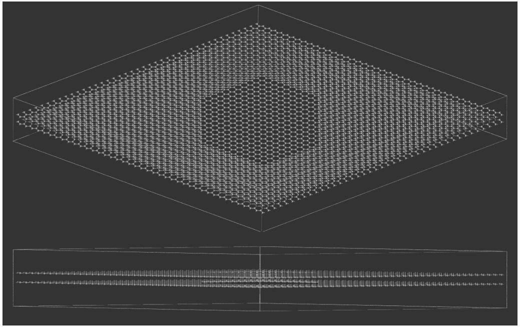
ATKPython & Simulating Nanomembranes

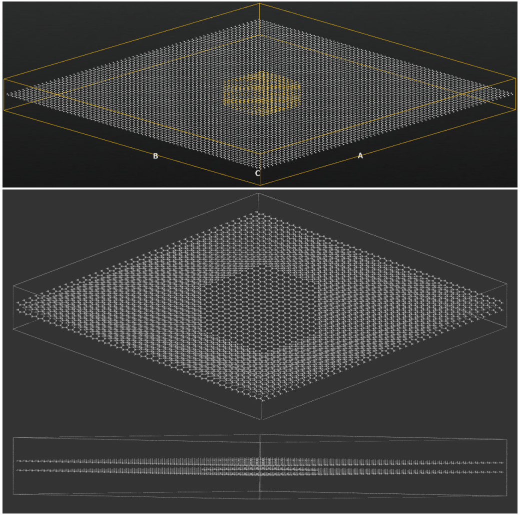
- Atomistic calculations





ATKPython & Simulating Nanomembranes

- Atomistic calculations
- HPC server cluster



ATKPython & Simulating Nanomembranes

- Atomistic calculations
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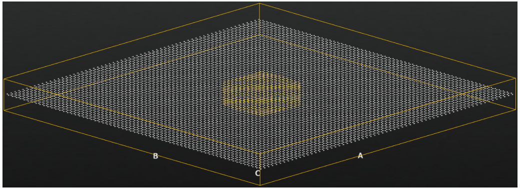
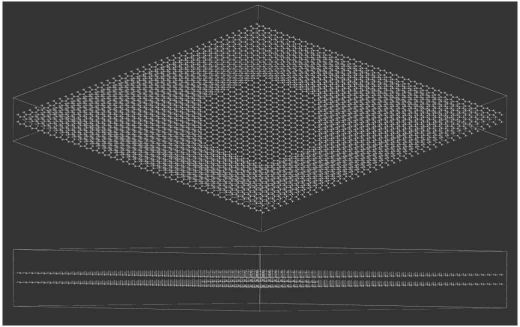
- Workflow
  1. Create configuration

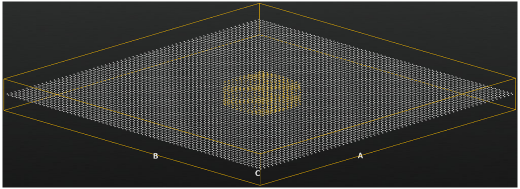


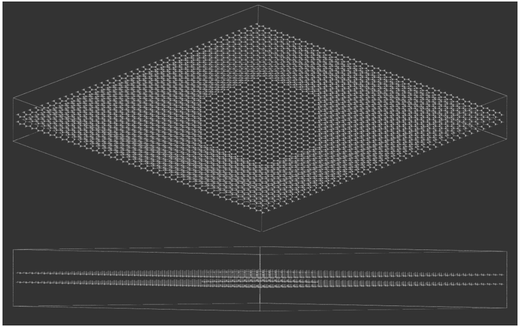


- Atomistic calculations
- HPC server cluster
- Workflow
  1. Create configuration
  2. Set potentials and optimise geometry

     - Intralayer: Tersoff-Brenner (2010)
     - Interlayer: Lennard-Jones:

$$V_{ij}(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$$





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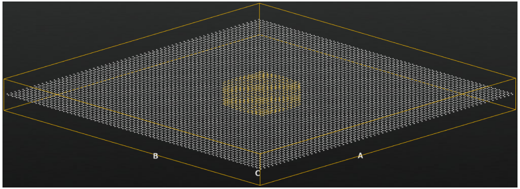

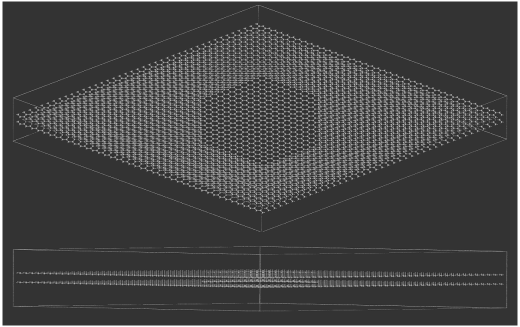

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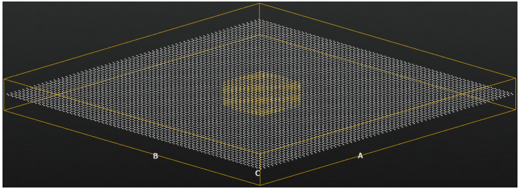

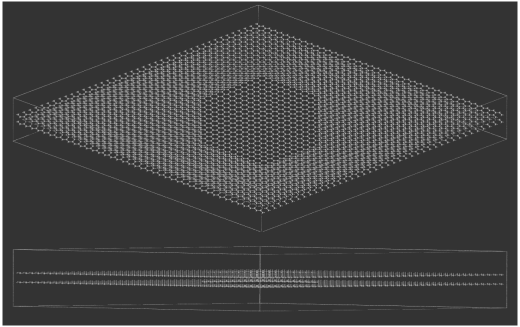

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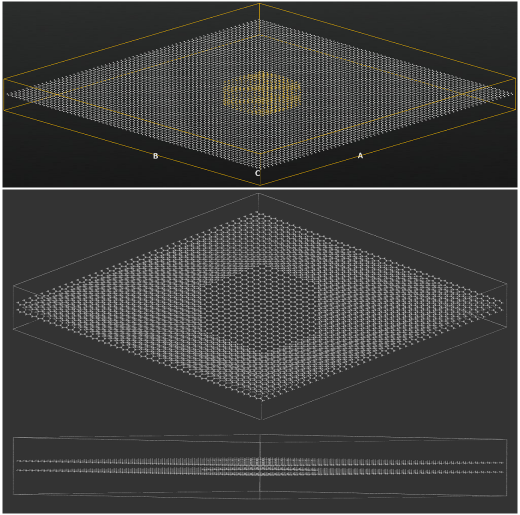

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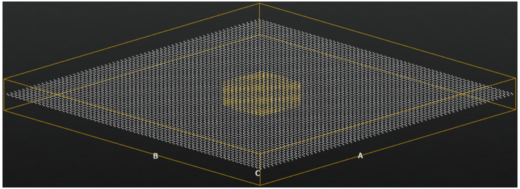
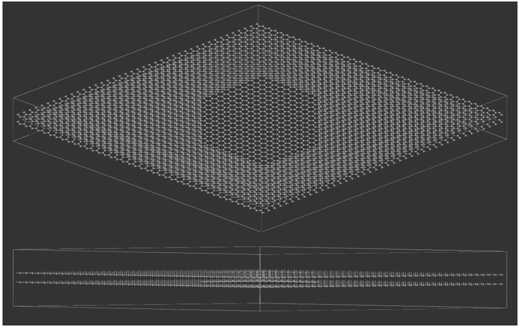
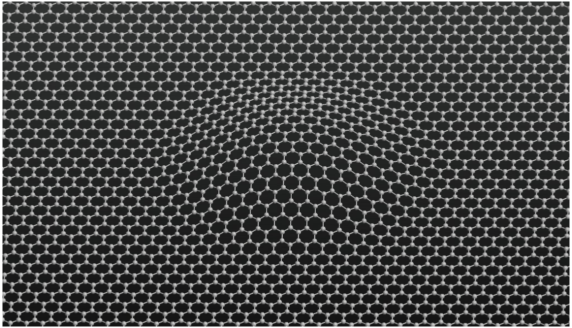
- ATKPython
- Matplotlib & Pyplot

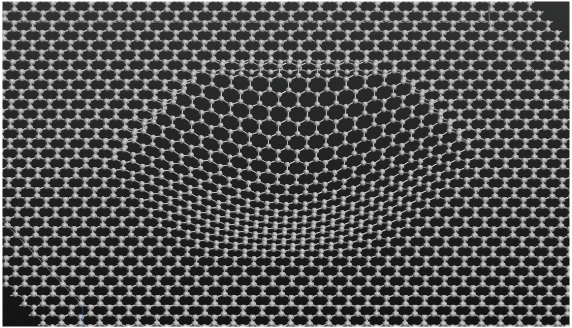




Visualising Modes

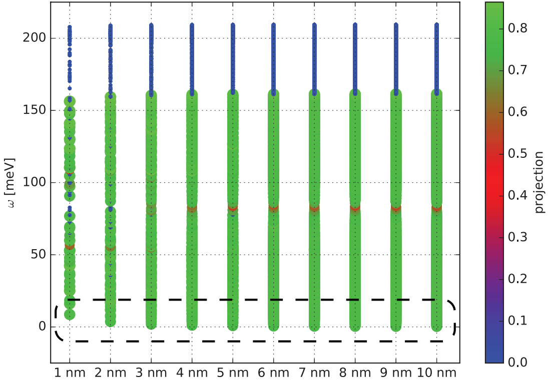


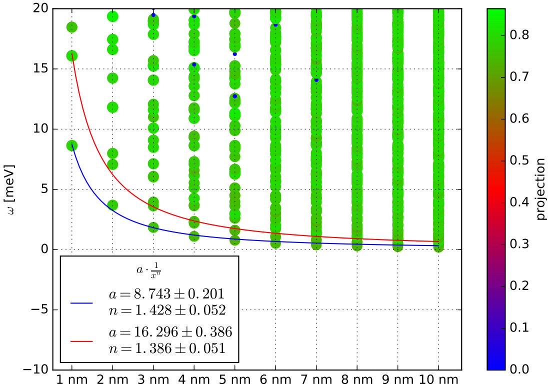
Clamped system



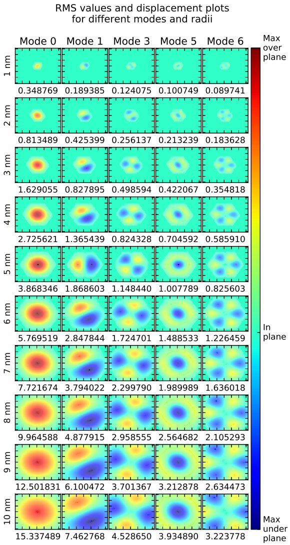
Supported system

Clamped System

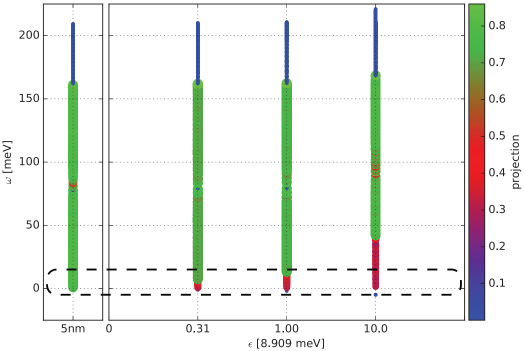


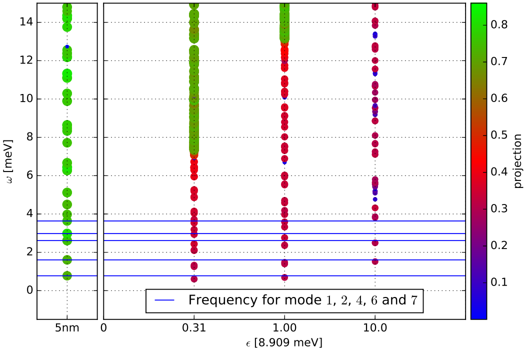


Frequencies vs size



Clamped vs Supported Systems





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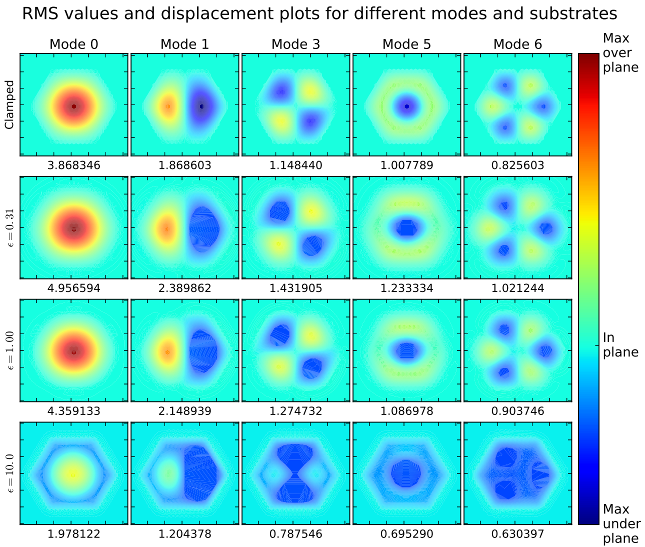
RMS values and displacement plots for different modes and substrates
Mode 0
Mode 1
Mode 3
Mode 5
Mode 6
Clamped
3.868346
1.868603
1.148440
1.007789
0.825603
$\epsilon = 0.31$
4.956594
2.389862
1.431905
1.233334
1.021244
$\epsilon = 1.00$
4.359133
2.148939
1.274732
1.086978
0.903746
$\epsilon = 10.0$
1.978122
1.204378
0.787546
0.695290
0.630397
Max over plane
In plane
Max under plane

Conclusion

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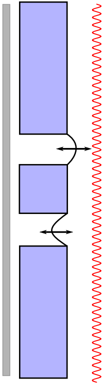

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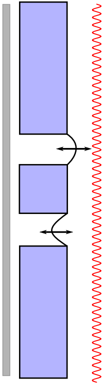
- SiO_2 Substrate: A good candidate



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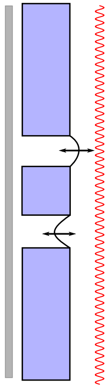
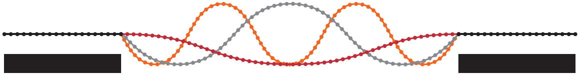
- Next step: Optimal Substrates, Molecular Dynamics, Hole Coupling, and Experimental testing



Questions



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