

Sharing Results with MD Showcase

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Molecular Dynamics Showcase



Goals:

Enable interactive exploration of published MD trajectories

Create a curated database of MD trajectories representing interesting results in the nano-bio area

Project Team:

- George Howlett, Developer, Purdue
- Chen-Yu Li, Graduate Student, UIUC
- Christopher Maffeo, Postdoctoral researcher, UIUC
- Lynn Zentner, Project manager, Purdue
- Michael McLennan, Senior Research Scientist, HUBzero team, Purdue
- John Stone, Senior Research Programmer, NIH Biotechnology Center, UIUC
- Aleksei Aksimentiev, Associate Professor, Physics, UIUC

Molecular Dynamics Showcase

⚙️ Terminate ▶ Keep for later

[Cite this work...](#)

[Download data for this view...](#)

[Upload trajectories and scripts...](#)

Interesting Parts of the Timeline

Interesting parts of the timeline can be highlighted and explained within the showcase.

In this example, a single strand of DNA diffuses through a nanopore on a thin, graphene surface.

- The first highlighted region shows the DNA adsorbing onto the graphene surface.
- The second highlighted region shows the DNA diffusing across the graphene surface and through the nanopore.

The single-strand DNA adsorbs to the graphene surface from bulk solution.

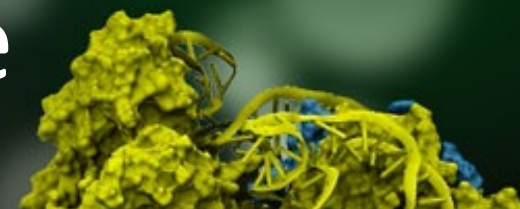
More To Explore

Storage (manage) | 2% of 10GB | 780 x 600

Status: Released
(2015)



Molecular Dynamics Showcase



Two typical uses

NANO LETTERS

Letter

pubs.acs.org/NanoLett

Assessing Graphene Nanopores for Sequencing DNA

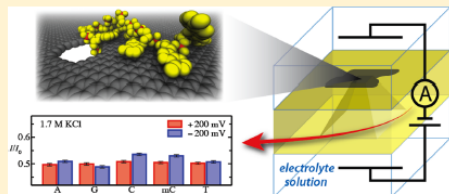
David B. Wells, Maxim Belkin, Jeffrey Comer, and Aleksei Aksimentiev*

Department of Physics, University of Illinois, 1110 W. Green St., Urbana, Illinois 61801, United States

Supporting Information

ABSTRACT: Using all-atom molecular dynamics and atomic-resolution Brownian dynamics, we simulate the translocation of single-stranded DNA through graphene nanopores and characterize the ionic current blockades produced by DNA nucleotides. We find that transport of single DNA strands through graphene nanopores may occur in single nucleotide steps. For certain pore geometries, hydrophobic interactions with the graphene membrane lead to a dramatic reduction in the conformational fluctuations of the nucleotides in the nanopores. Furthermore, we show that ionic current blockades produced by different DNA nucleotides are, in general, indicative of the nucleotide type, but very sensitive to the orientation of the nucleotides in the nanopore. Taken together, our simulations suggest that strand sequencing of DNA by measuring the ionic current blockades in graphene nanopores may be possible, given that the conformation of DNA nucleotides in the nanopore can be controlled through precise engineering of the nanopore surface.

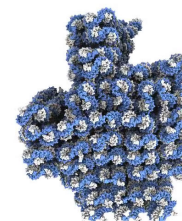
KEYWORDS: Nanopore, graphene, molecular dynamics, biosensors, nucleic acids, ionic current, next generation DNA sequencing



The elastic-network guided simulation worked extremely well. In just 2 nanoseconds of simulation, the DNA conformation approached a conformation consistent with the cryo-EM reconstruction (see [trajectory](#) on nanoHUB). Such a short simulation can be performed on a workstation. To validate the all-atom simulation protocol, the elastic-network guided structure was submerged in solvent and simulated for ~150 ns. The structure was [seen](#) to be stable.

MD simulation accurately captures subtle structural features of DNA origami. For example, the characteristic [chickenwire pattern](#) observed in experiment emerges in our simulations. Unusual motifs, such as the [left-handed psuedo-helix](#) are realistically modeled. Hence, if atomically-detailed structure prediction is needed, MD simulation is the method of choice. Setup your own origami structure prediction simulation [here!](#)

The ["pointer" object](#) was simulated via all-atom MD for 200 ns, starting from an idealized configuration of straight DNA helices. The DNA helices were seen to spread apart quickly as a global twist developed. The root-mean-squared-deviation from the psuedo-atomic structure derived from cryo-electron microscopy was seen to decrease monotonically, approaching 1 nm.



0:18

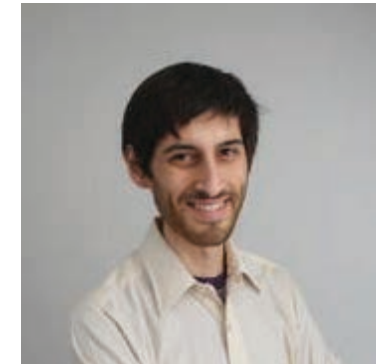
Link from a pdf

Link from a webpage





Chen-Yu Li



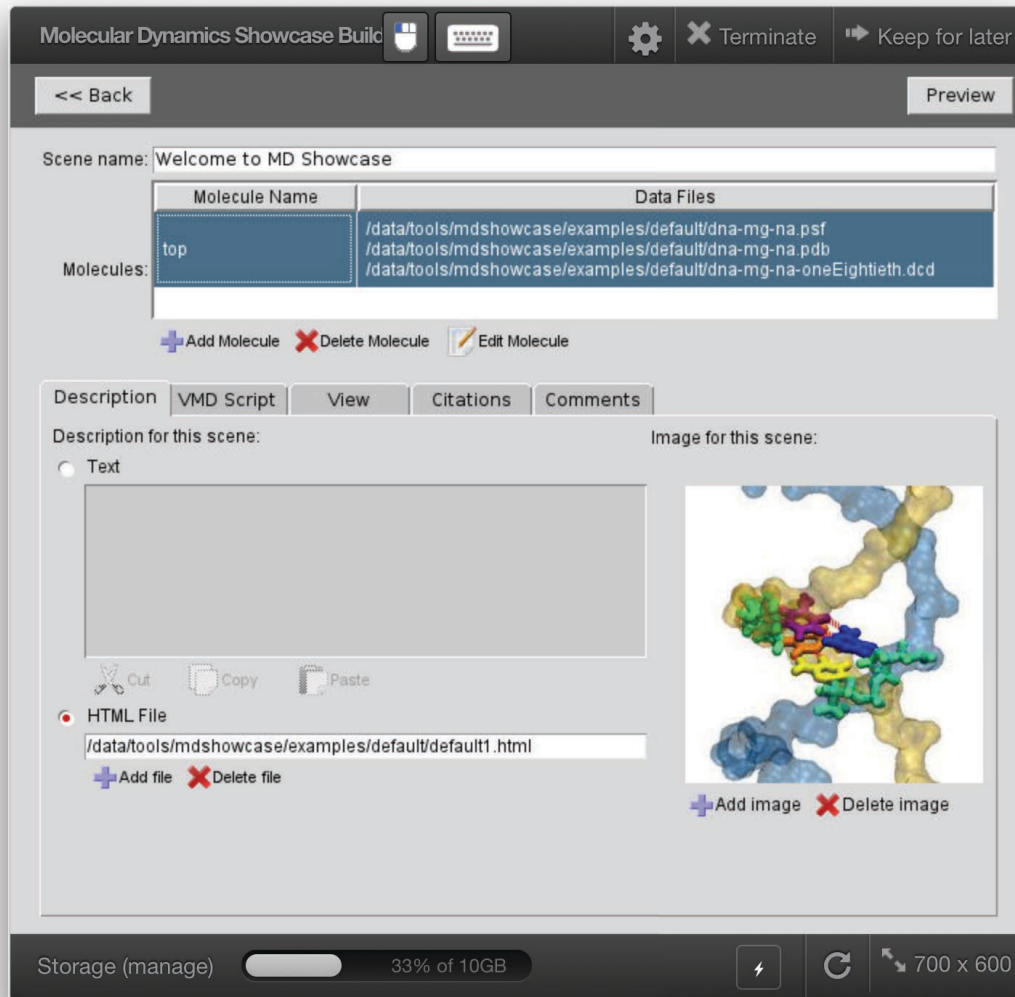
Chris Maffeo

DEMO:

<http://bionano.physics.illinois.edu/node/214>

MD Showcase Builder: a tool for making showcases

nanoBIO NODE



Built-in examples

Intuitive interface

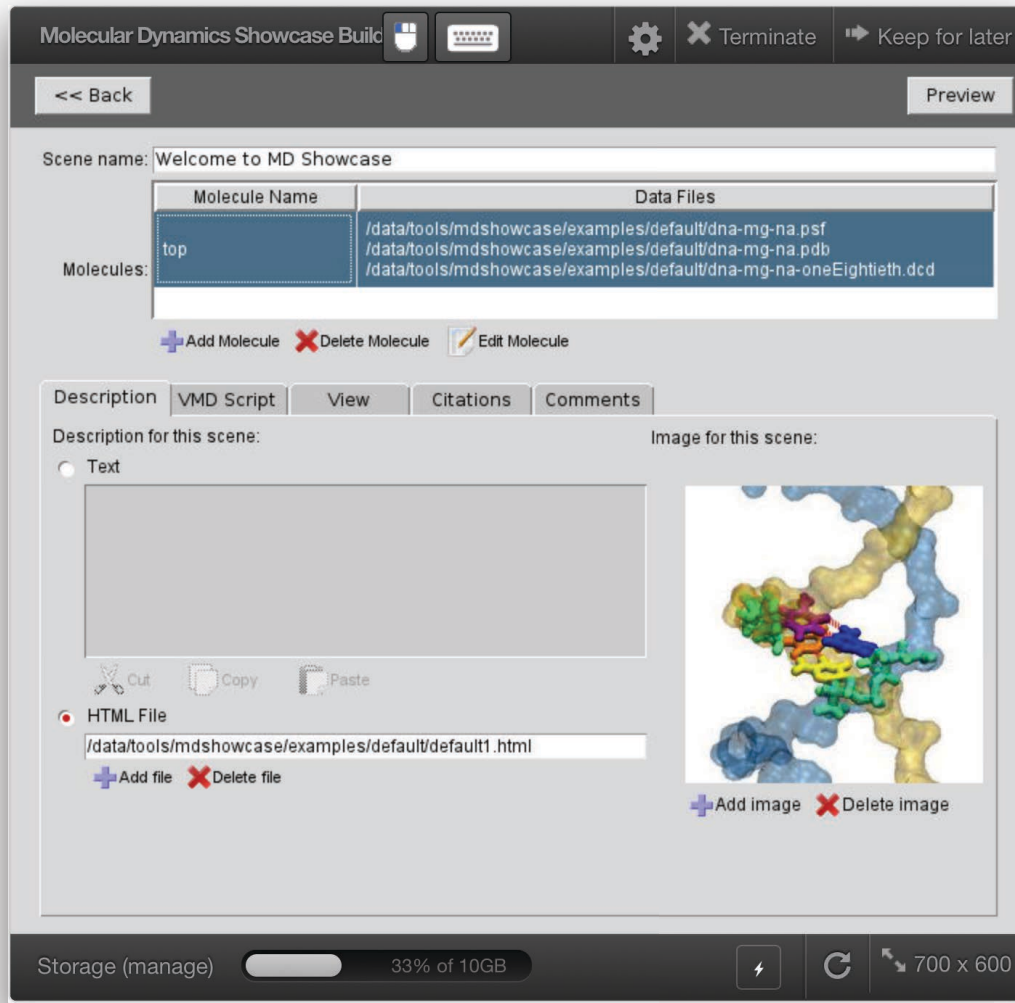
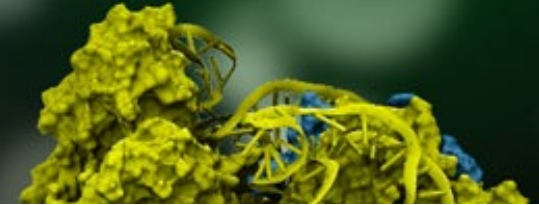
Advanced molecular
graphics options

Support for binary
images

Status: released



MD Showcase Builder: a tool for making showcases



- upload/download showcase files
- built-in examples
- easy editing of scripts and showcase information:
 - scene title, description, thumbnail image, trajectory data, citations
 - VMD representation script (adapted from saved VMD session)
 - view script for moving the camera
 - playback settings: speed & smoothness
 - comments
- built-in VMD previewer
- sharing and publishing

Status: released



Builder features: Built-in showcase previewer



Allows users to see their changes to the showcase from within the builder

Preview Mode Exit Preview

[Cite this work...](#)

[Download data for this view...](#)

Welcome to MD Showcase


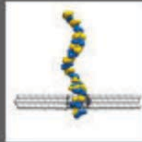
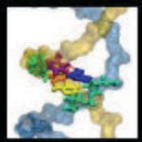
This application helps you view the data produced by molecular dynamics simulators such as [NAMM](#). It uses the [VMD](#) visualization engine developed with NIH support by the Theoretical and Computational Biophysics group at the Beckman Institute, University of Illinois at Urbana-Champaign.

This example shows two nucleotide base pairs stacked within a DNA molecule. Use the player controls to view the evolution of this molecule as a function of time.

Use the following controls to change the view:

- When this control is active, you can click and drag in the molecular view area to rotate the molecule. If you let go while quickly dragging the molecule, you can cause it to spin in place.
- When active, click and drag to move the molecule up/down or left/right.
- When active, click and drag up to zoom in, or drag down to zoom out.
- When active, click on an atom to see information about it. Shift-click on another atom to measure the distance between atoms. Shift-click on another

More To Explore

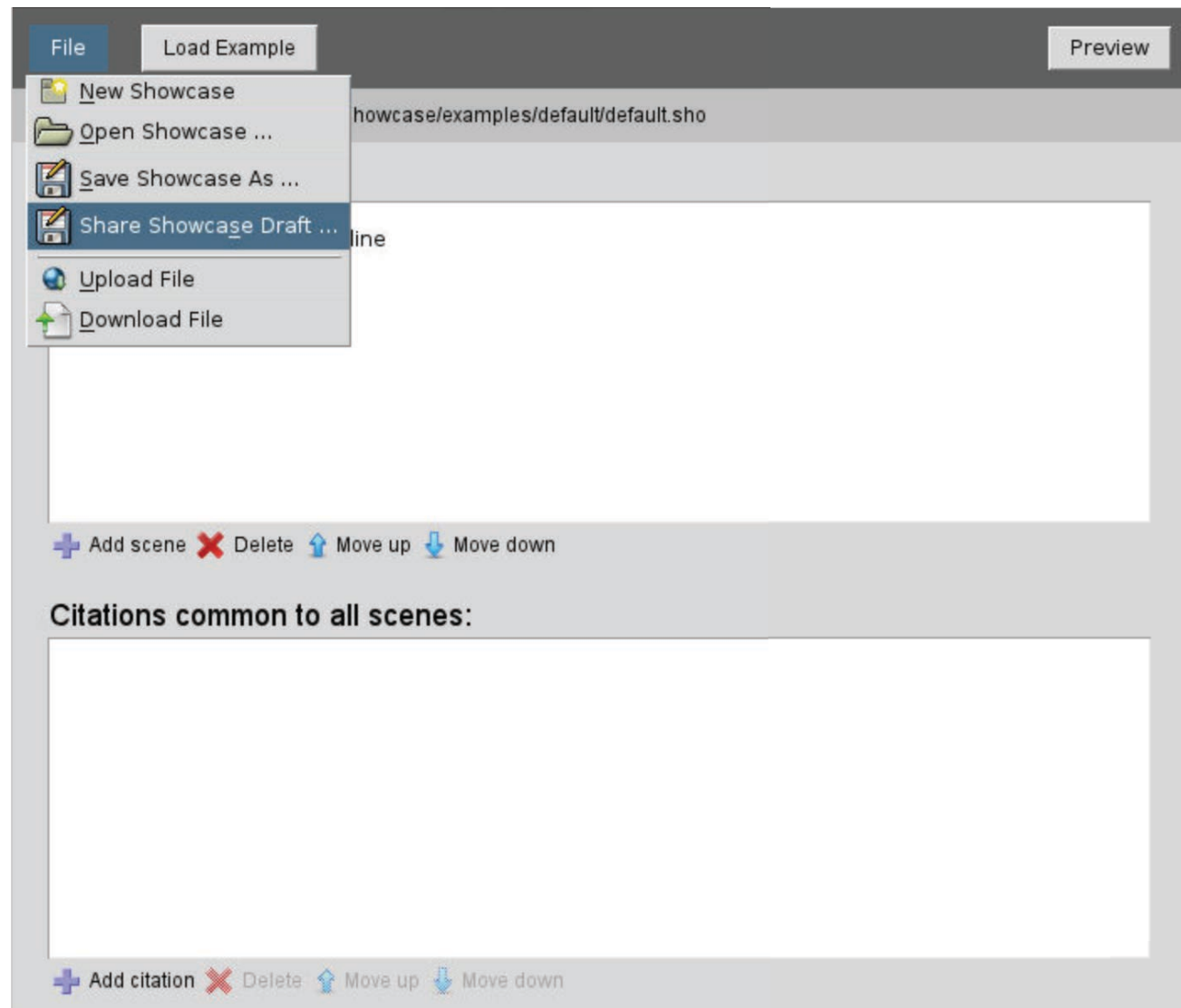




Builder features: sharing showcases

Sharing transfers a showcase to a location accessible to nanoHUB users and provides an html link


Subsequent publishing associates each scene with a doi



Step-by-step tutorial



The builder tutorial demonstrates how the builder is used in detail (30 pages!)



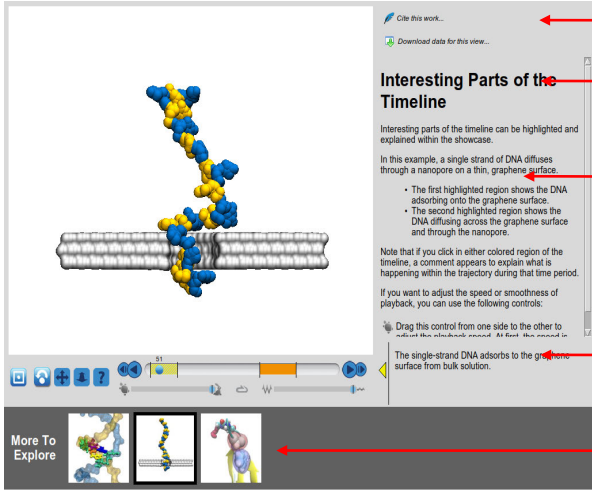
HUB



Hub Technology Group
Rosen Center for Advanced Computing


Showcase Scene

A *scene* has several components.

- Title
- Description
- Preview image
- Trajectory data files.
 - PDB, PSF, DCD, ...
- VMD script
- Comments (optional)
- View settings
- Citations (optional)







Demonstration



Chrome File Edit View History Bookmarks People Window Help

nanoHUB.org - Home nanoHUB.org - Group: MD nanoHUB.org - Resources

https://nanohub.org

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SIMULATE

HUNDREDS OF CUTTING-EDGE TOOLS TO PROPEL YOUR RESEARCH