Sharing Results with MD Showcase

Aleksei Aksimentiev
Department of Physics, University of Illinois

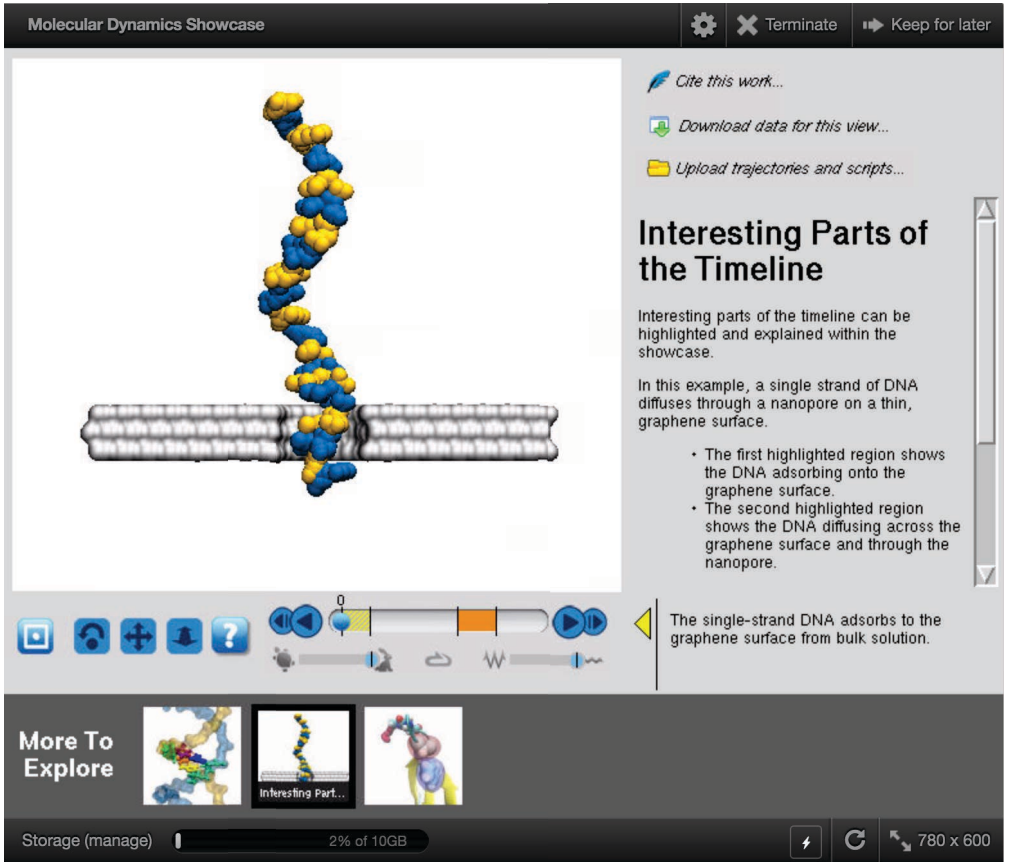
nanoBIO NODE

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

Status: Released (2015)

nanoBIO NODE

Molecular Dynamics Showcase

Two typical uses

NANO LETTERS

Letter

pubs.acs.org/NanoLett

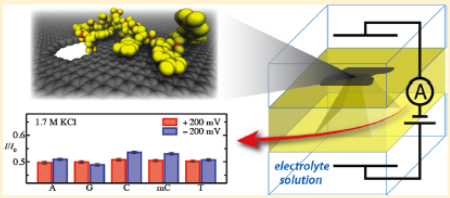
Assessing Graphene Nanopores for Sequencing DNA

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.

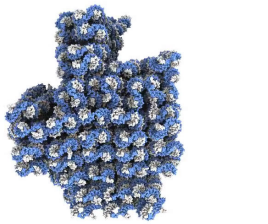


KEYWORDS: *Nanopore, graphene, molecular dynamics, biosensors, nucleic acids, ionic current, next generation DNA sequencing*

Link from a pdf

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.

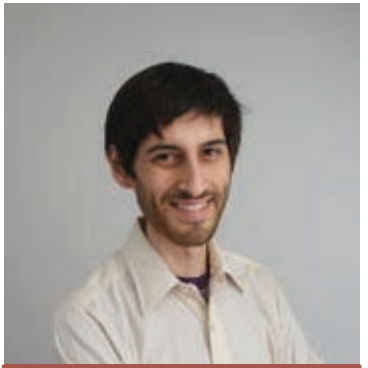
MD simulation accurately captures subtle structural features of DNA origami. For example, the characteristic chickenwire pattern observed in experiment emerges in our simulations. Unusual motifs, such as the left-handed psuedo-helix are realistically modeled. Hence, if atomically-detailed structure prediction 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.

Link from a webpage

Chen-Yu Li



Chris Maffeo

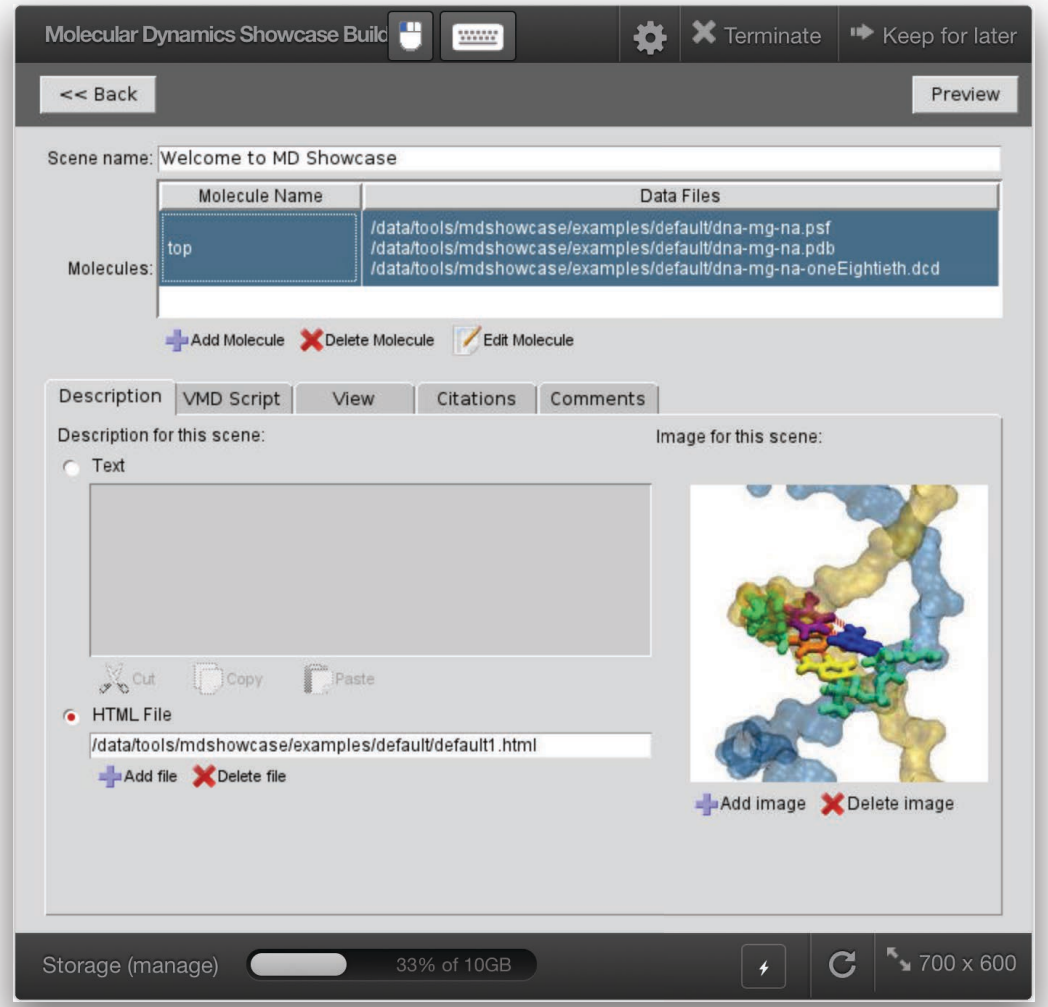
DEMO:

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

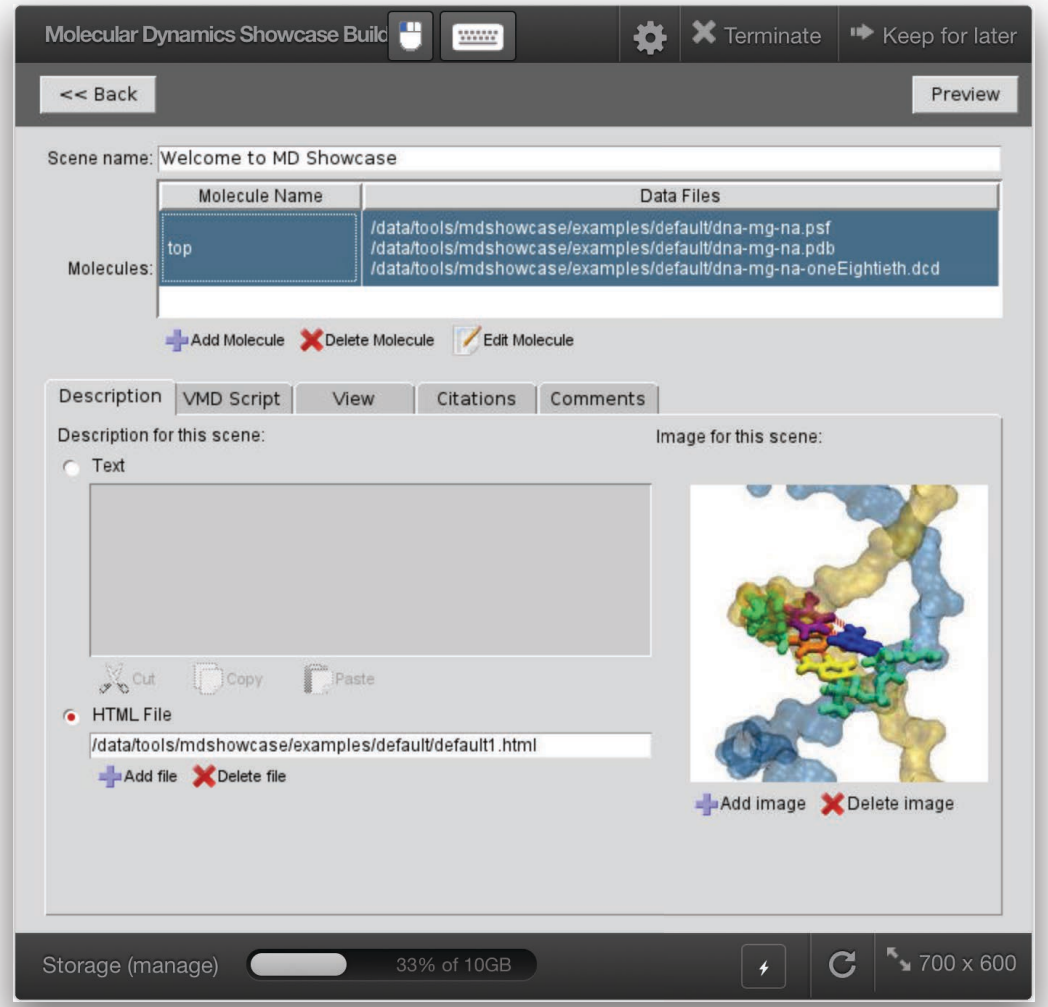
Support for binary images

Status: released

MD Showcase **Builder:**

a tool for making showcases

nanoBIO NODE



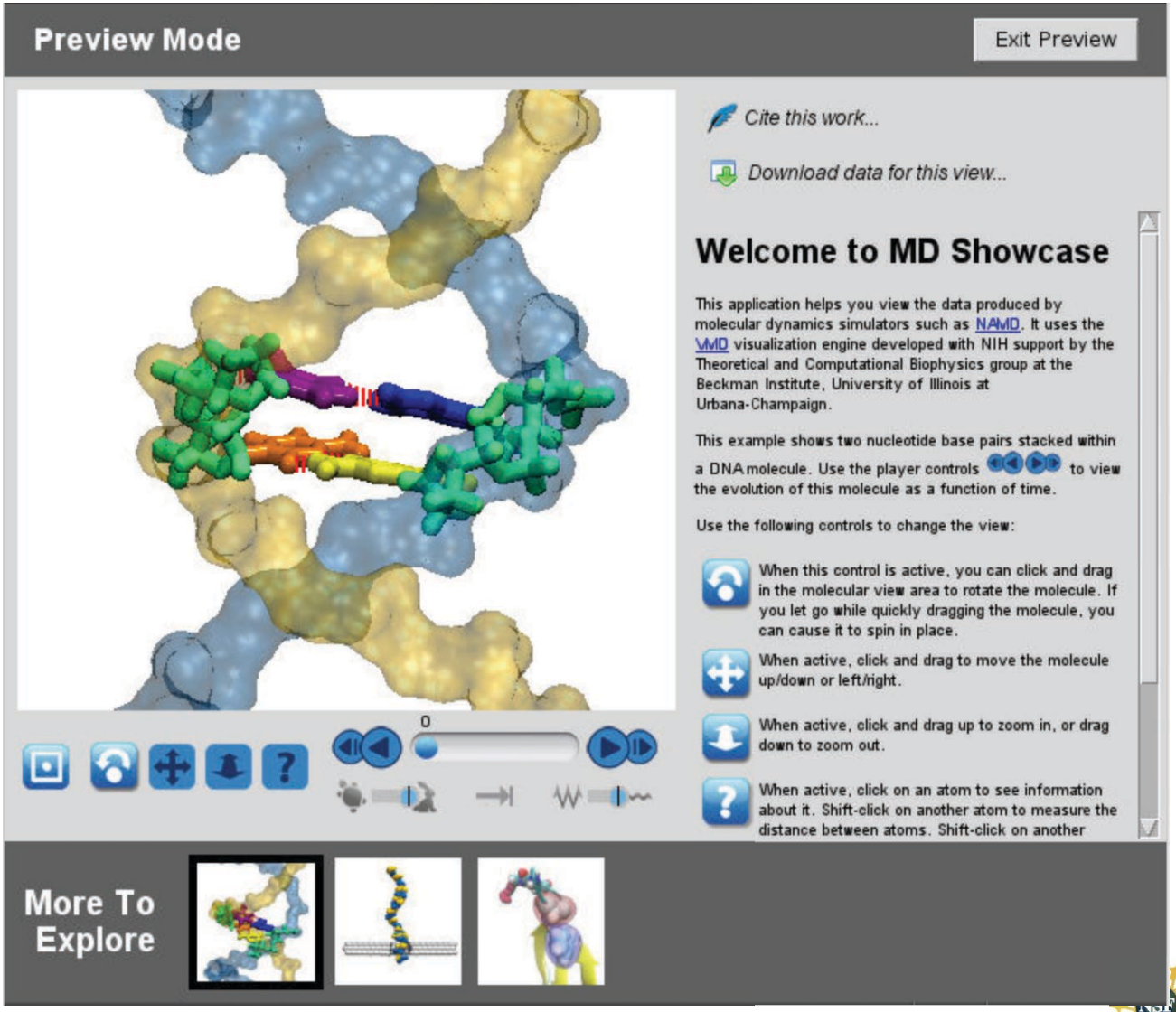
- upload/download showcase files
- built-in examples
- easy editing of scripts and showcase information:
  - scene title, description, thumbnail image, trajectory data, citations
  - VMD representation script (adapted from saved VMD session)
  - view script for moving the camera
  - playback settings: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

Status: released

Builder features: Built-in showcase previewer

nanoBIO NODE

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

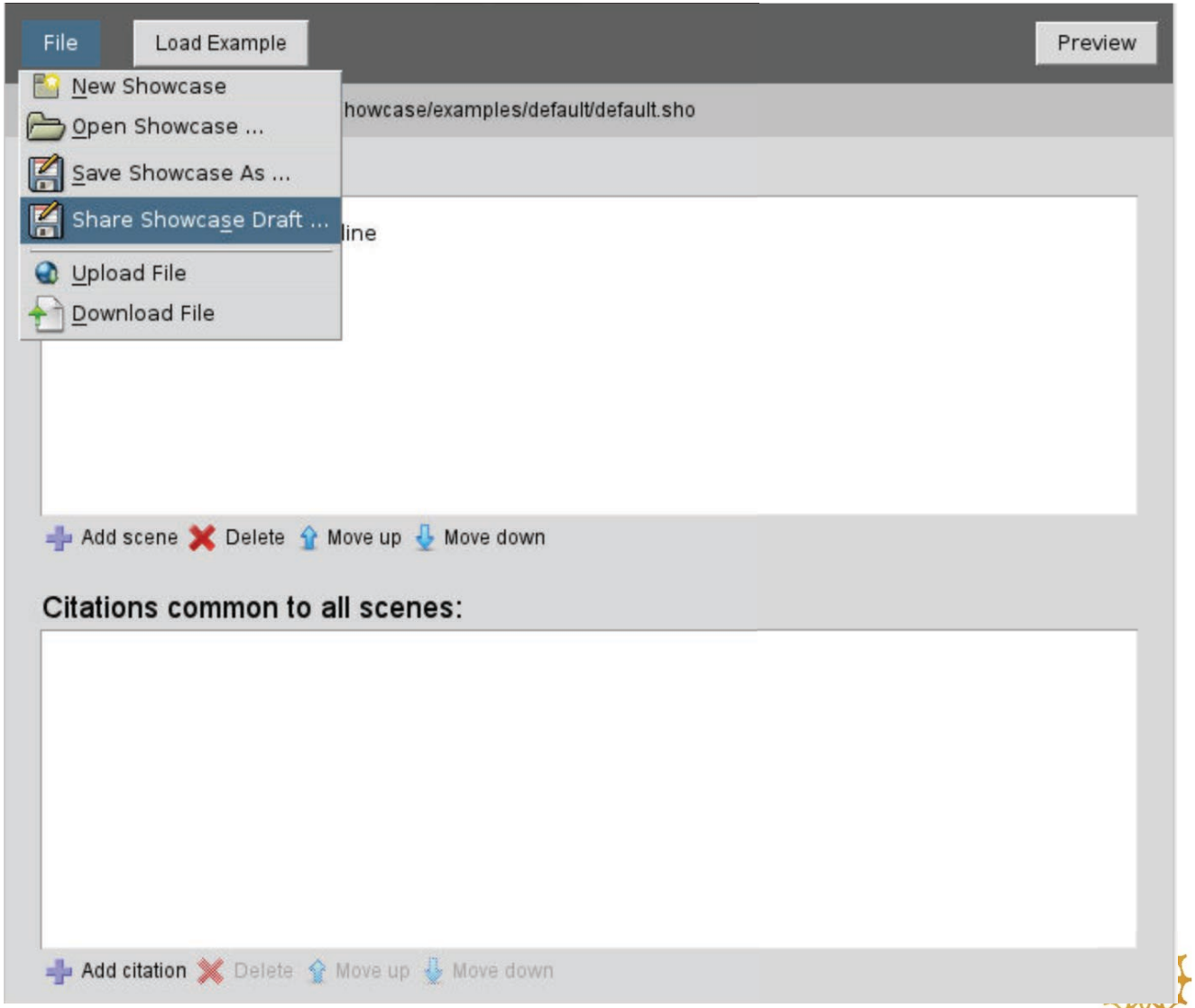


Builder features: sharing showcases

nanoBIO NODE

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!)

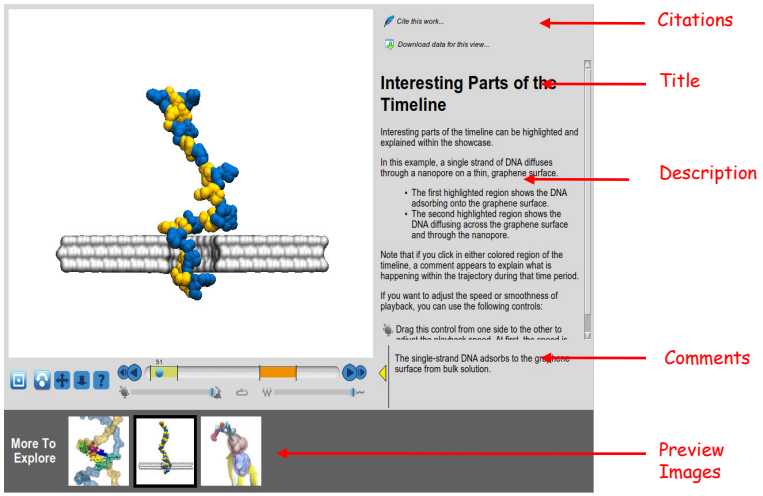
HUB

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)



PURDUE UNIVERSITY ITaP

Demonstration