Title: Modeling of RNA Nanotube using Molecular Dynamics Simulation

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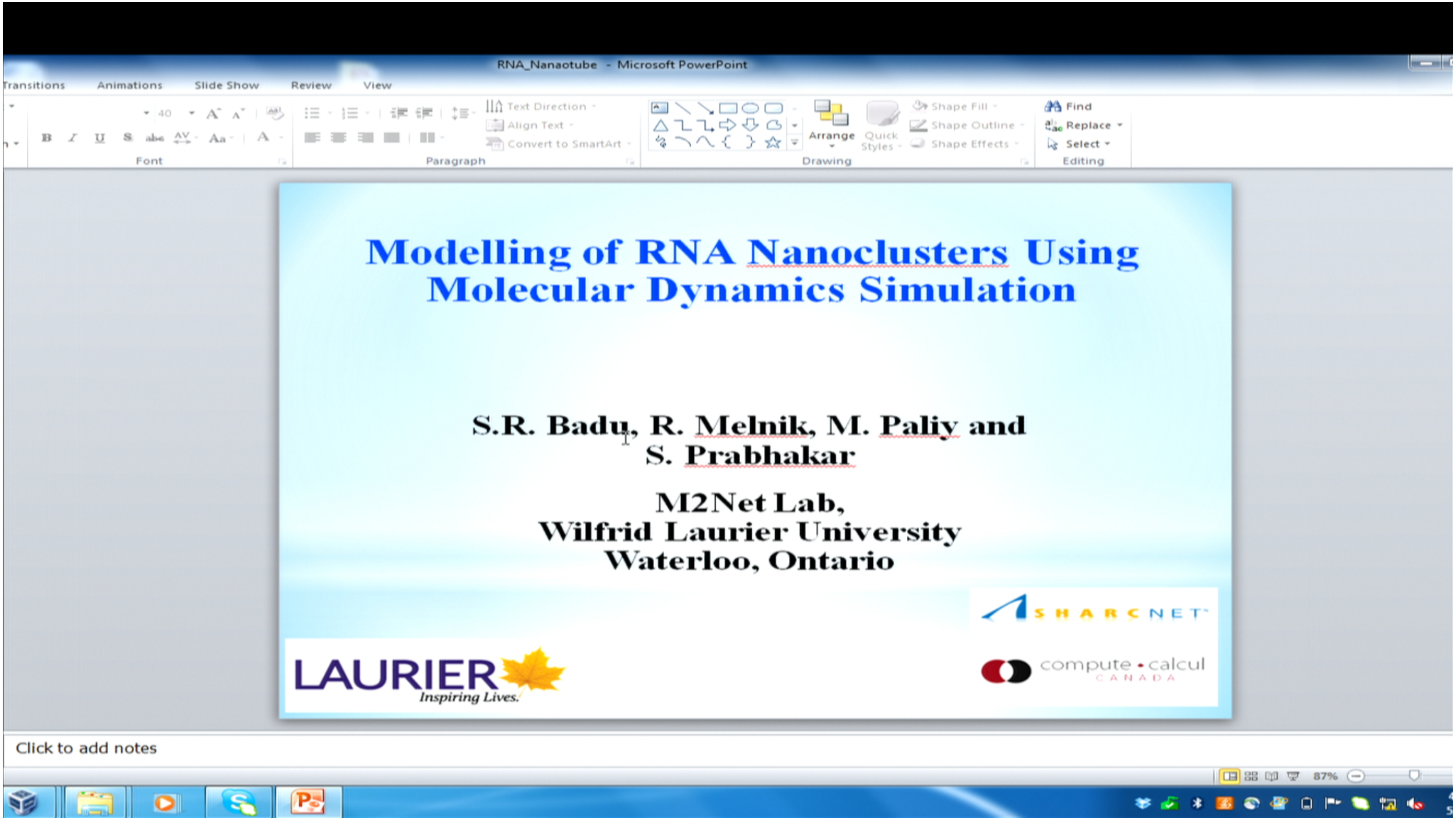
URL: http://pirsa.org/14050058

Abstract: We construct the novel RNA nanpclusters- the RNAnanotubes made of several nanorings. We study the struc-tural properties (i.e. the Root Mean Square Deviation (RMSD)the radius of gyration and radial distribution function) ofRNA nanotube up to the size of about 20nm in physilogicalsolution that can be used for drug delivery into human body.We model RNA nanotube by utilizing molecular dynamicssimulation method implemented in NAMD and VMD. Thepatterns of energy and temperature variations of the systemsare also discussed. Furthermore we study the number of ionsaround the tube as a function of time at a particular temper-ature. We find that if the temperature increases the numberof ions increases within certain distance of the tube. We re-port that the number of ions within a certain distance aroundthe tubes decrease in quenched run. This indicates that someions evaporate with decrease in temperature a


RNA_Nanaotube - Microsoft PowerPoint
Transitions
Animations
Slide Show
Review
View
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Editing
Text Direction
Align Text
Convert to SmartArt
Arrange
Quick Styles
Shape Fill
Shape Outline
Shape Effects
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Replace
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Modelling of RNA Nanoclusters Using Molecular Dynamics Simulation
S.R. Badu, R. Melnik, M. Paliy and S. Prabhakar
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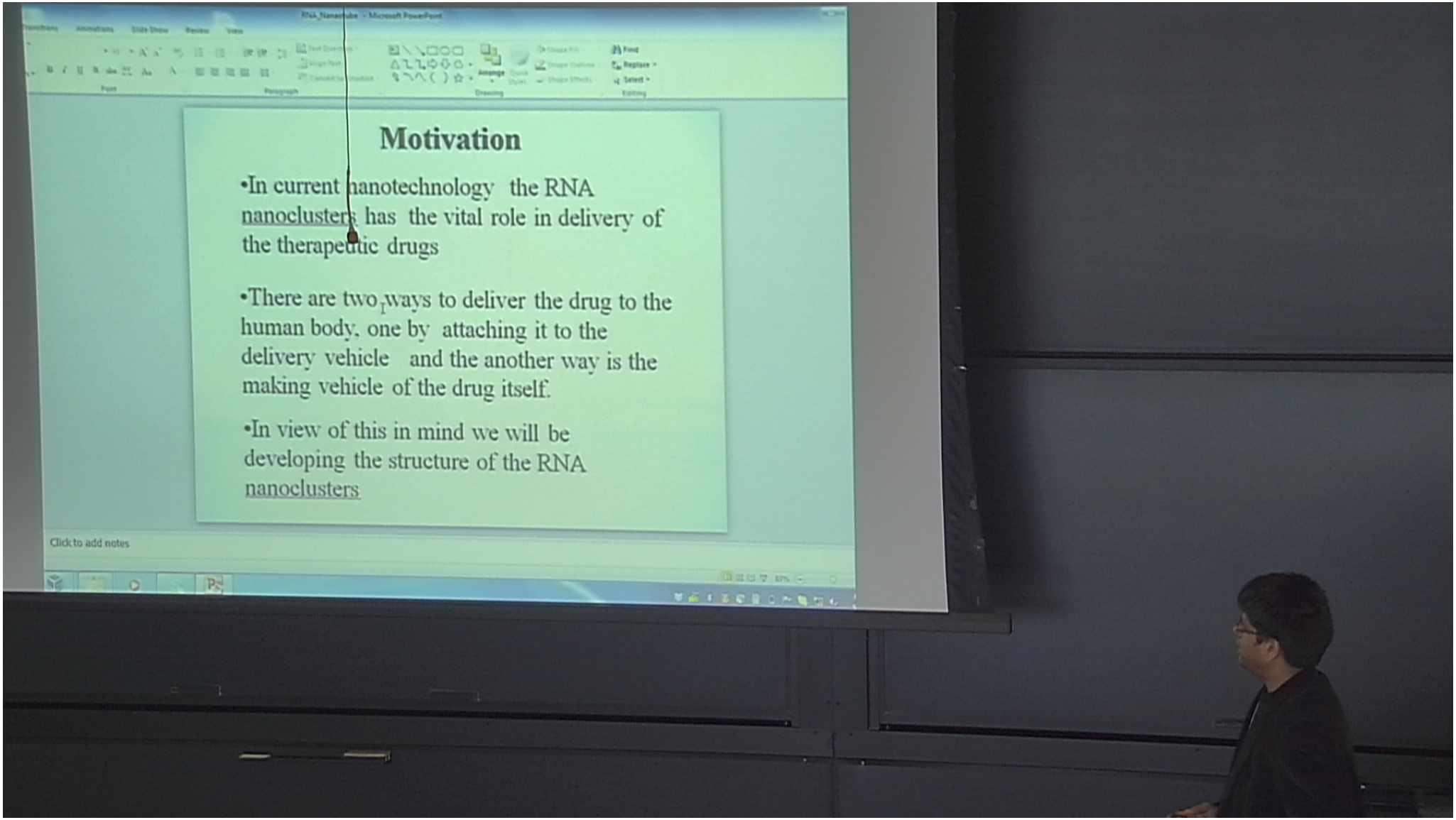
Motivation
•In current nanotechnology the RNA nanoclusters has the vital role in delivery of the therapeutic drugs
•There are two ways to deliver the drug to the human body, one by attaching it to the delivery vehicle and the another way is the making vehicle of the drug itself.
•In view of this in mind we will be developing the structure of the RNA nanoclusters
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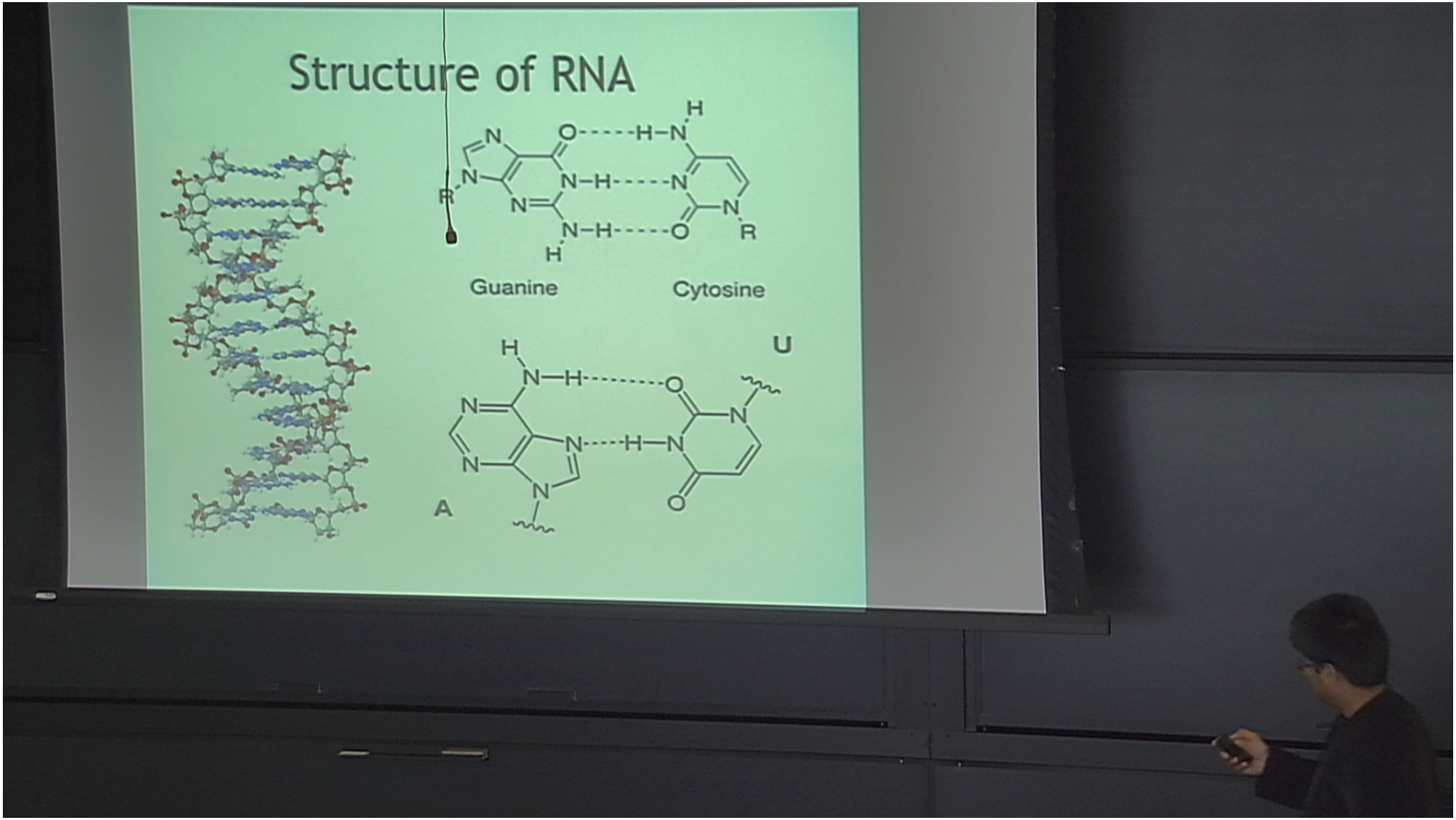
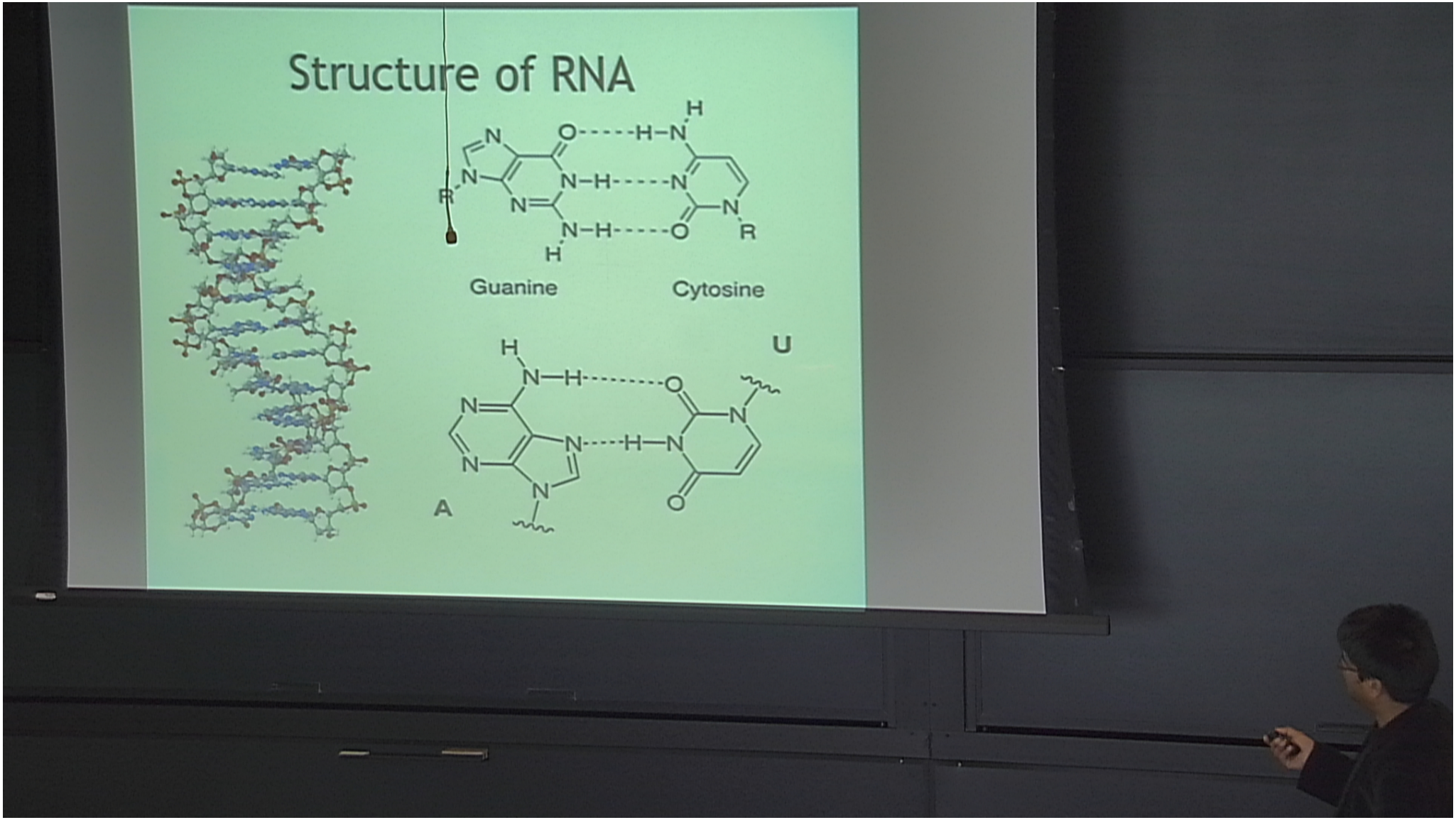

Structure of RNA
Guanine
Cytosine
A
U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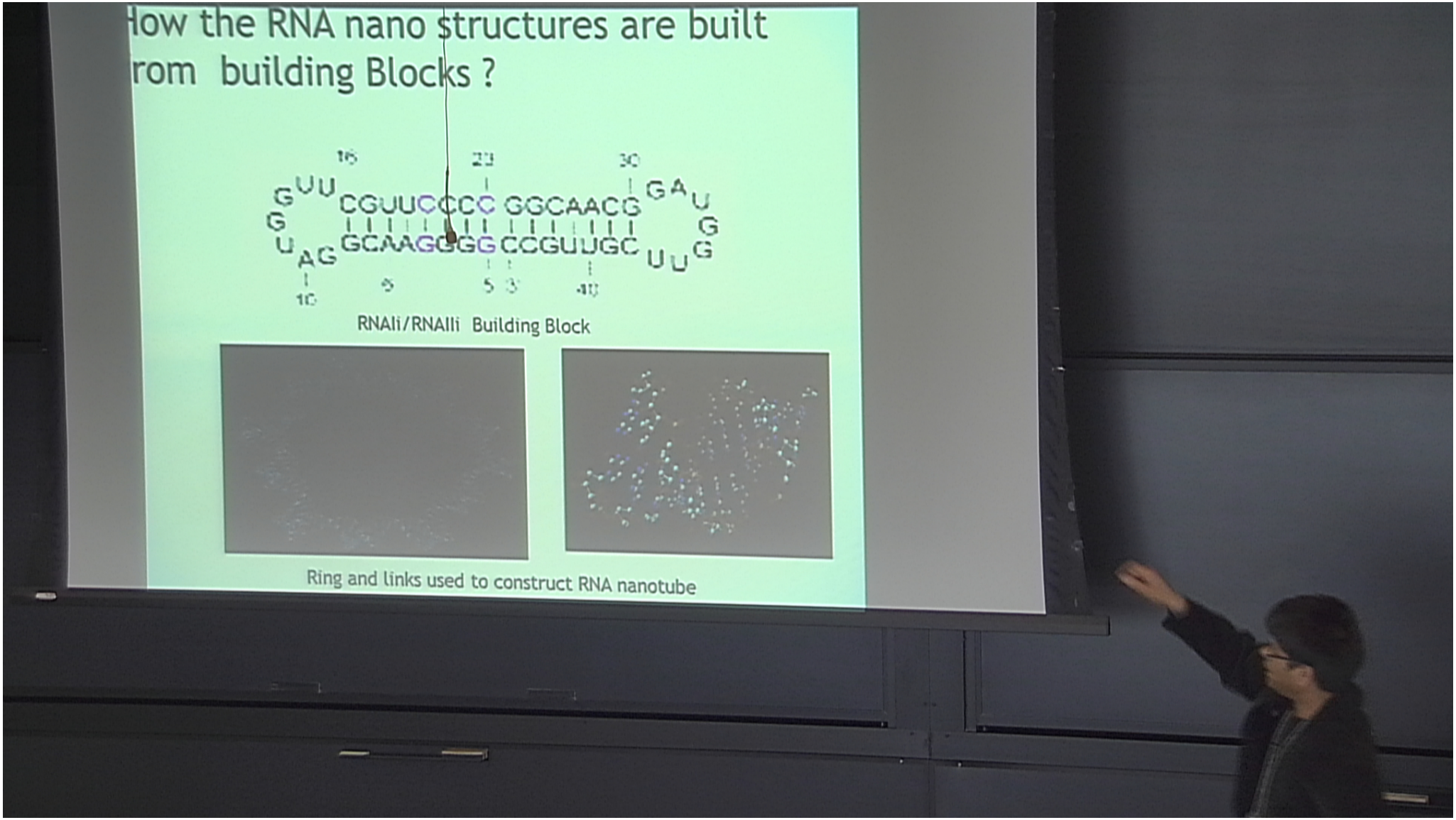
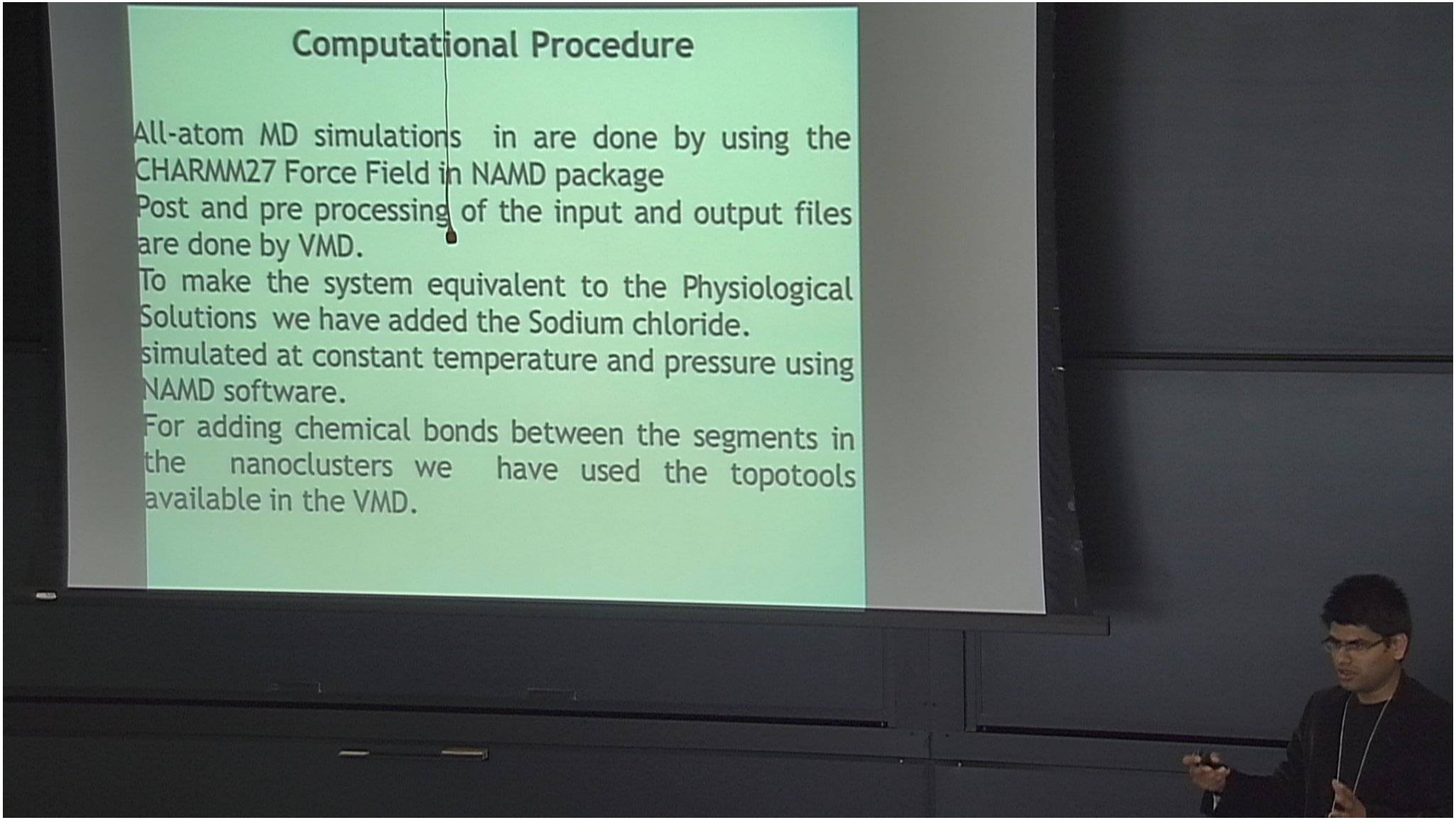
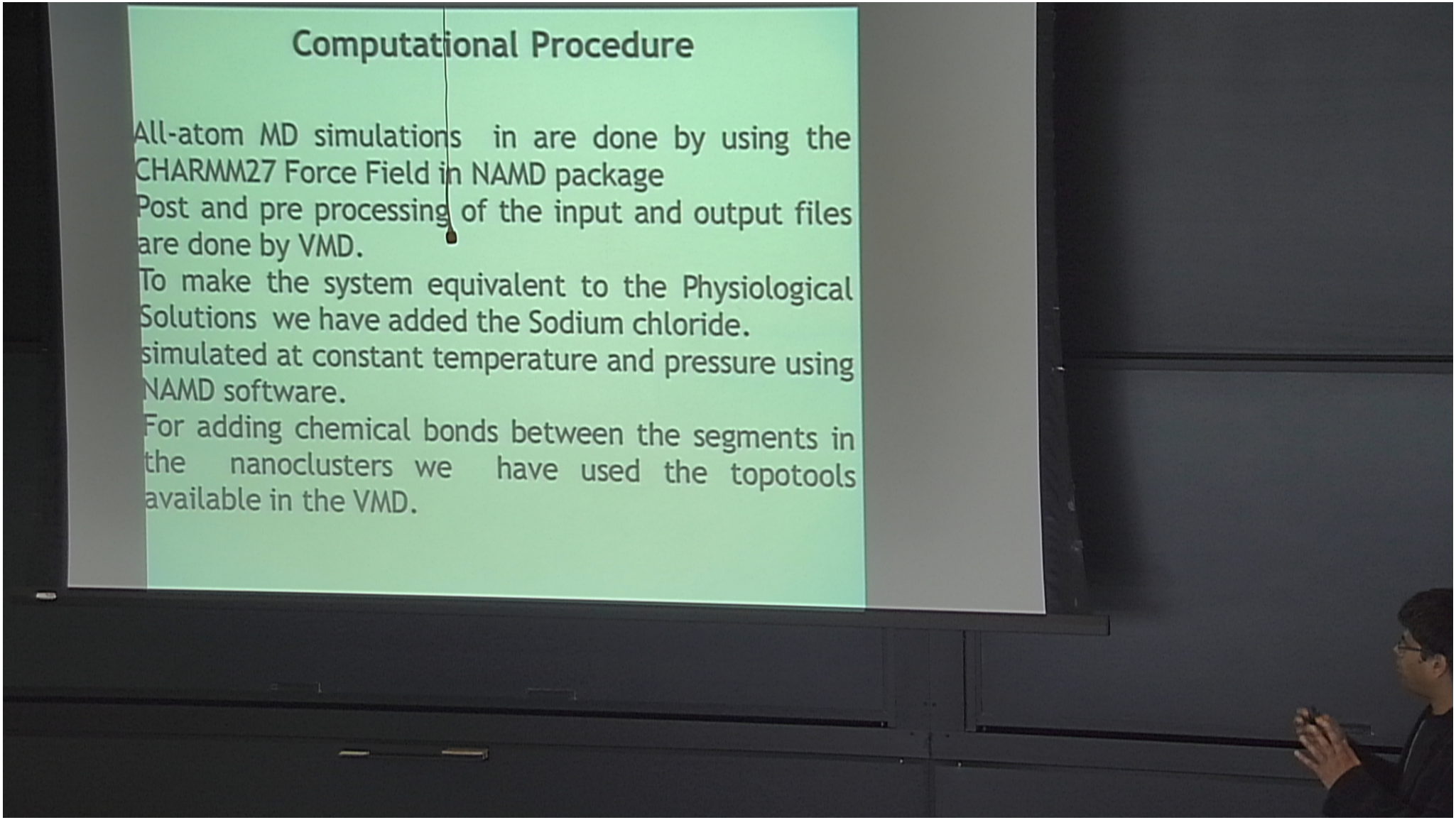

How the RNA nano structures are built
rom building Blocks ?
RNAi/RNAIi Building Block
Ring and links used to construct RNA nanotube


(a)
(b)
Ring and Ring with the link


Computational Procedure
All-atom MD simulations in are done by using the CHARMM27 Force Field in NAMD package
Post and pre processing of the input and output files are done by VMD.
To make the system equivalent to the Physiological Solutions we have added the Sodium chloride.
simulated at constant temperature and pressure using NAMD software.
For adding chemical bonds between the segments in the nanoclusters we have used the topotools available in the VMD.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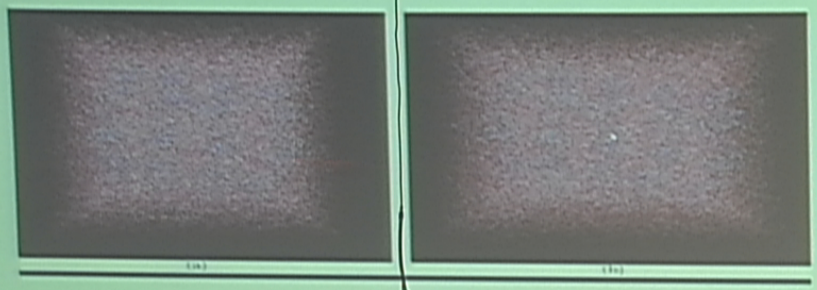
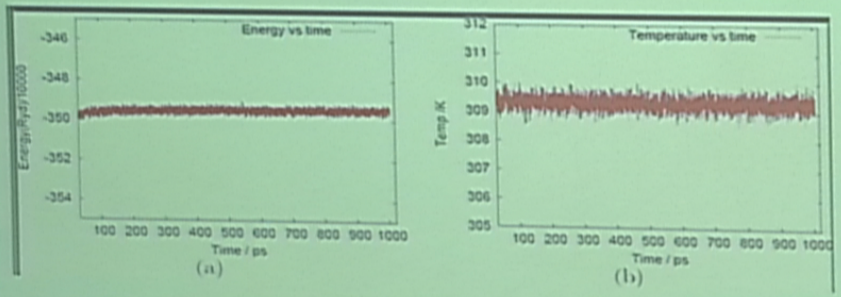
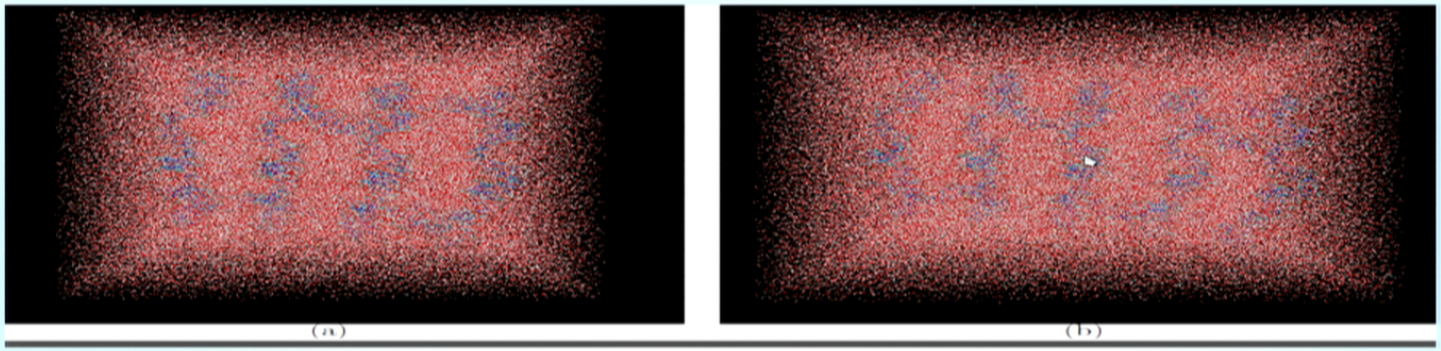


MD generated RNA nanotube in water and salt to match the physiological solutions (a) tube with 4 rings (b) tube with 5 nanorings.



(a) Energy and (b) Temperature vs. simulation time for the all-atom MD simulation of 2 ring RNA nanotube in water and salt.



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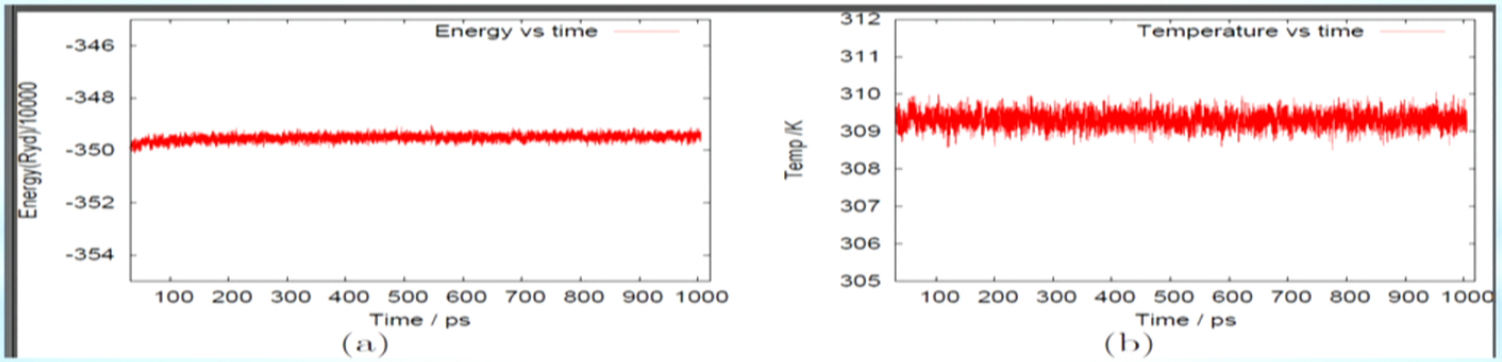

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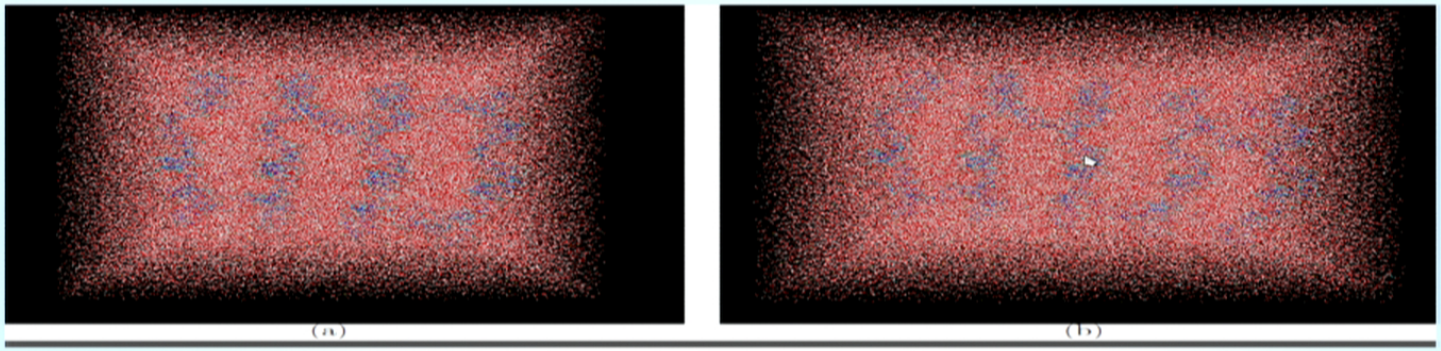

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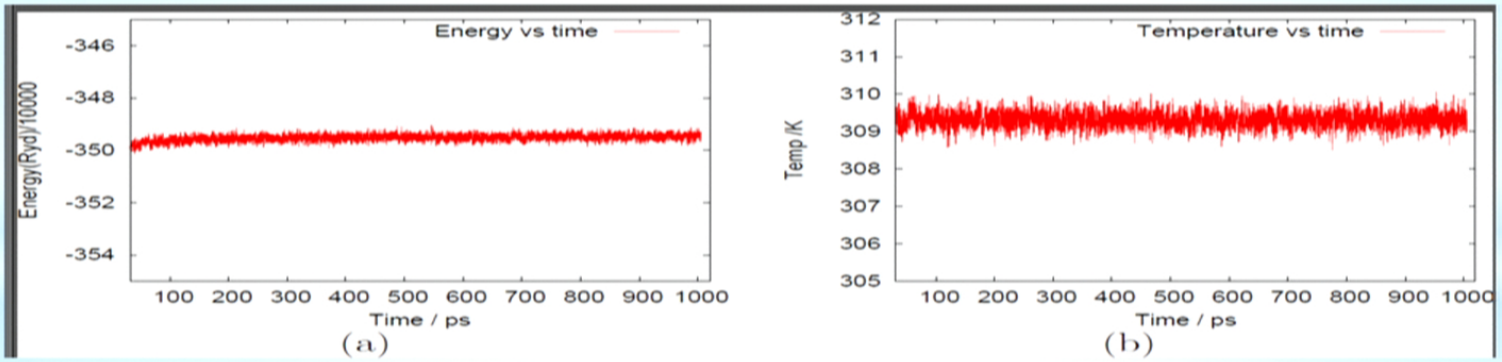

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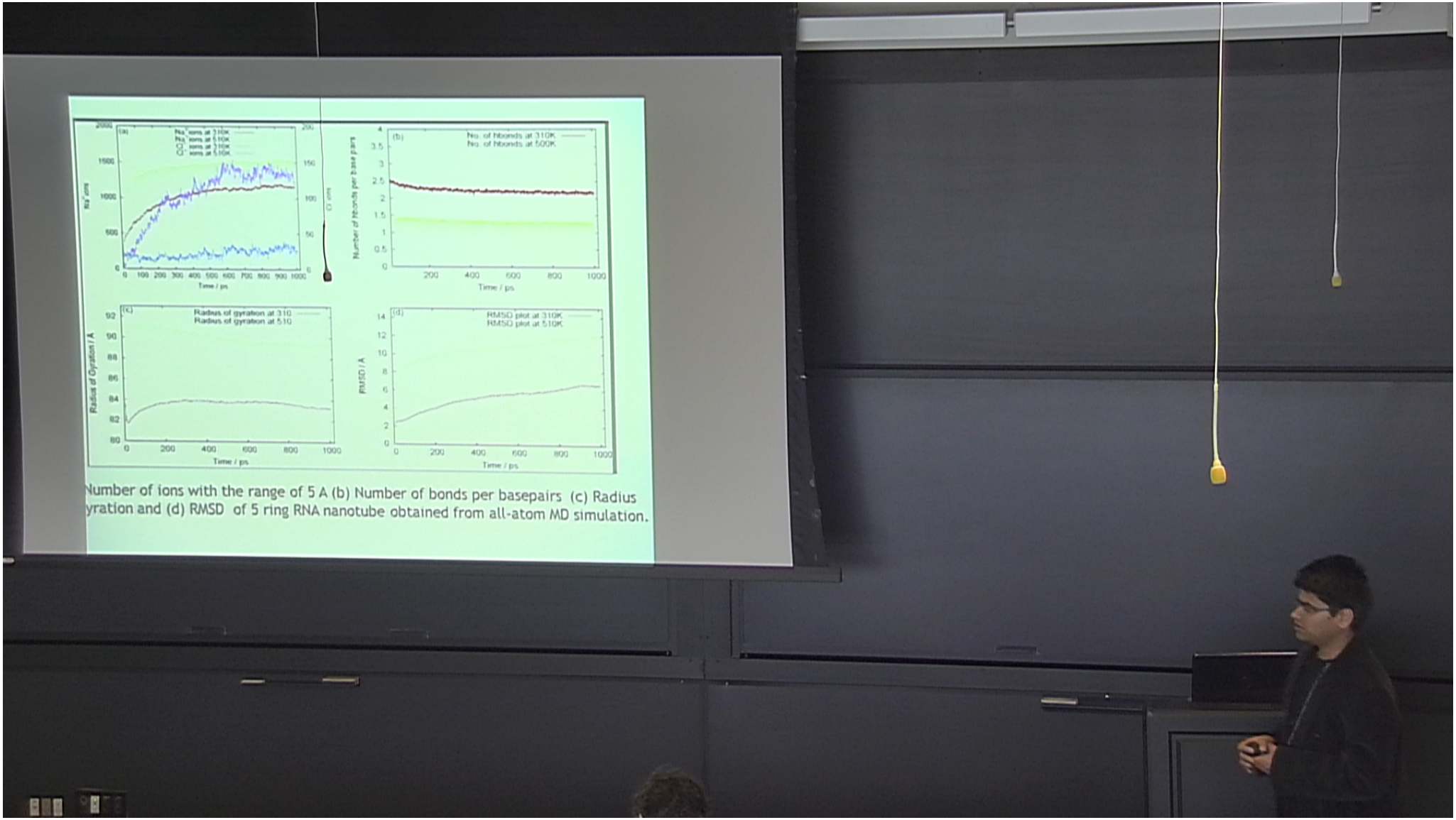
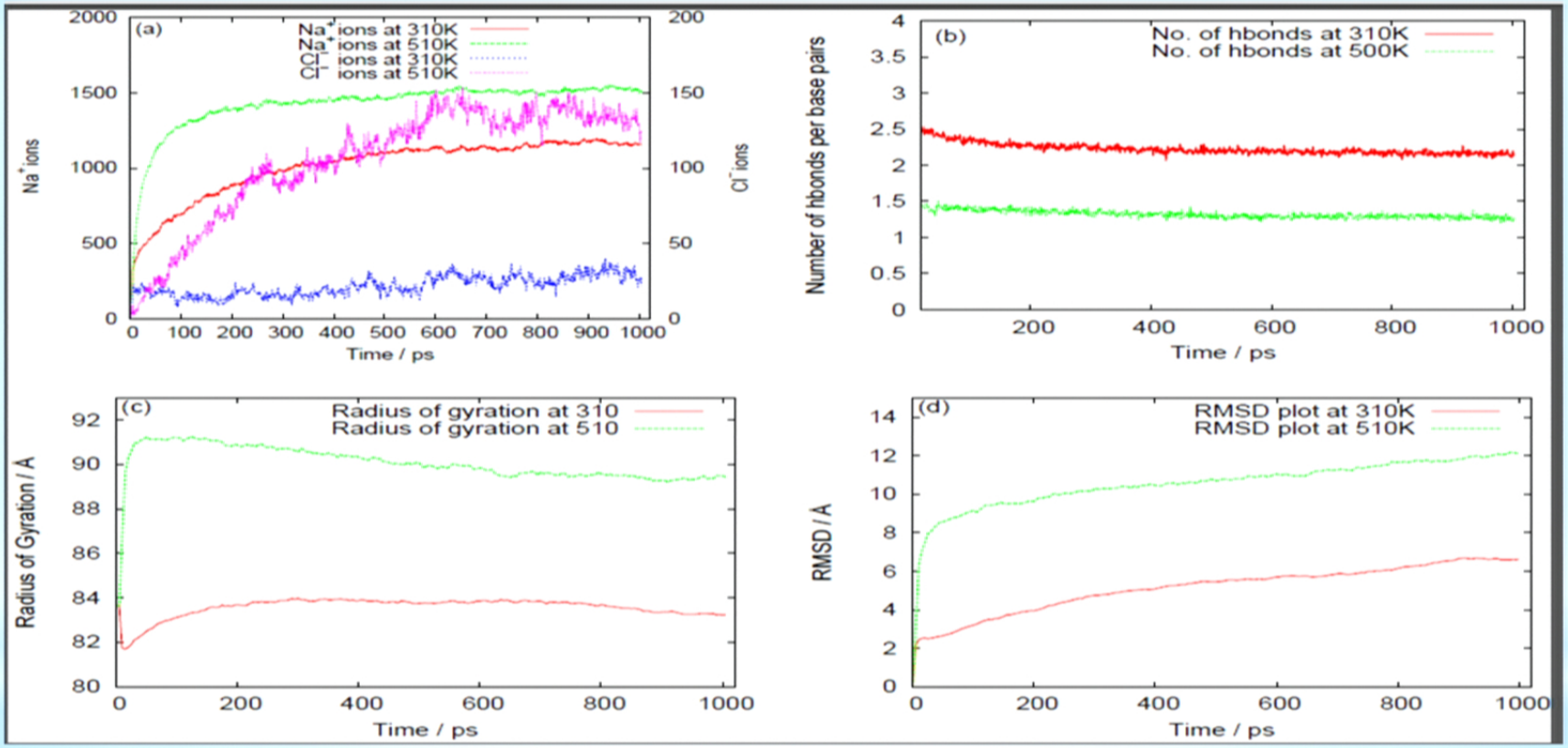


Number of ions with the range of 5 A (b) Number of bonds per basepairs (c) Radius yration and (d) RMSD of 5 ring RNA nanotube obtained from all-atom MD simulation.



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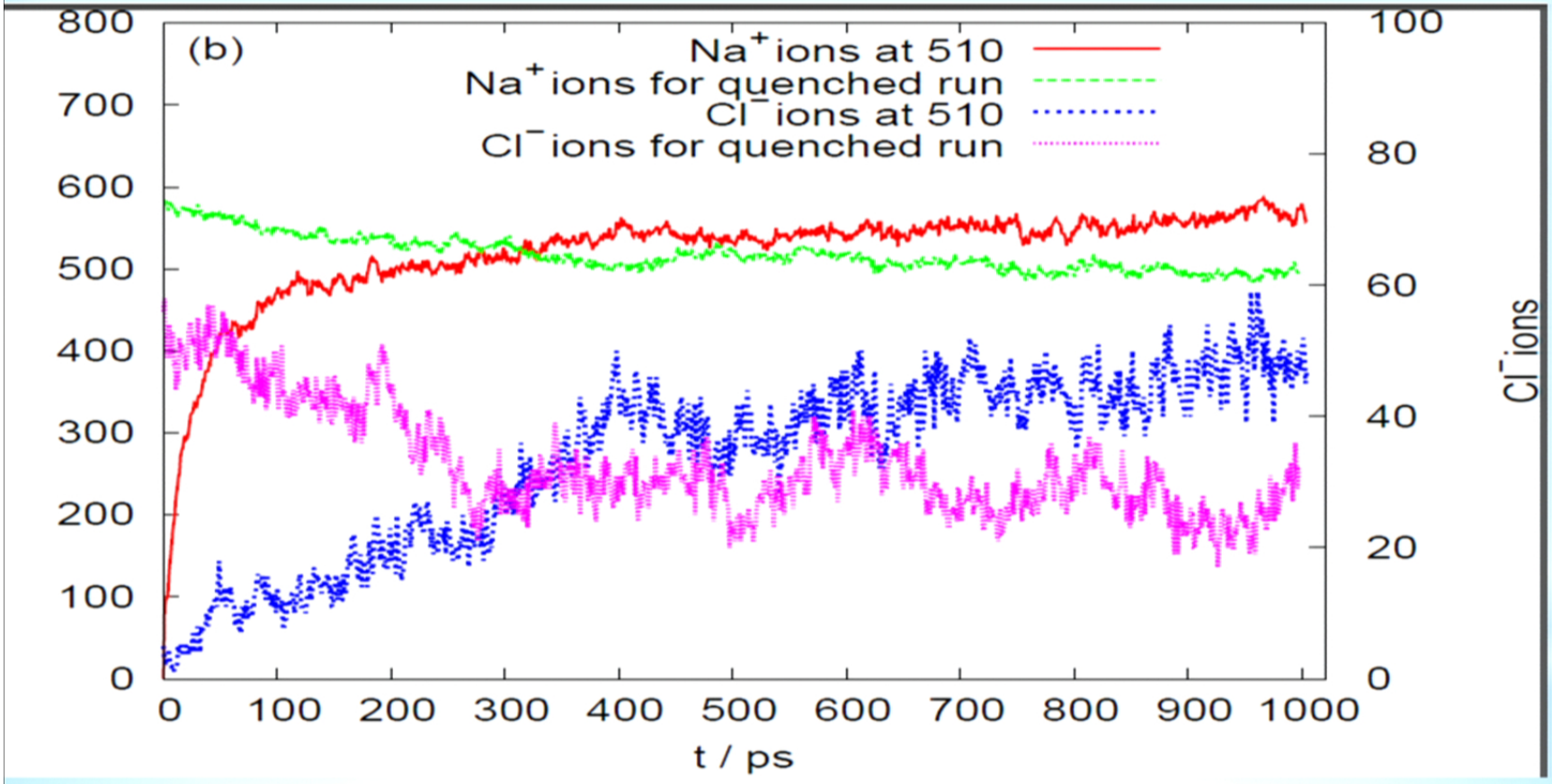
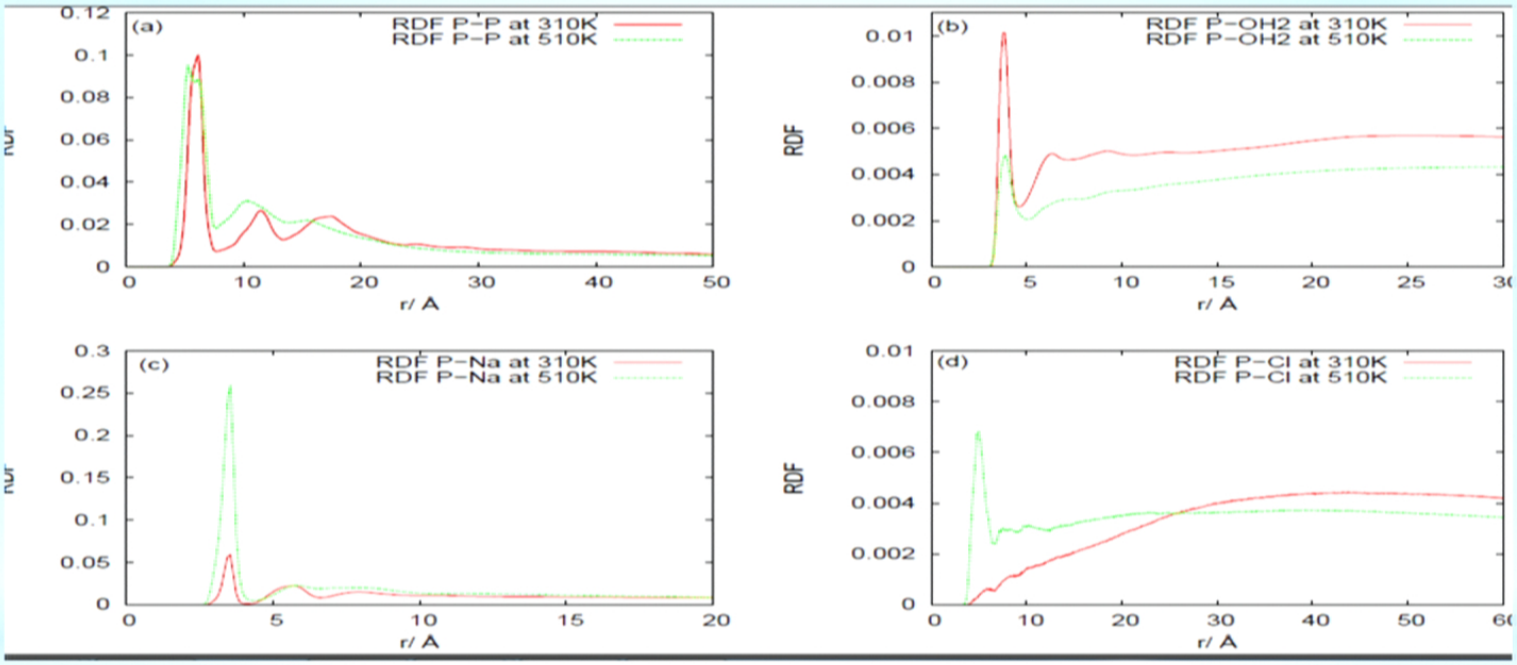


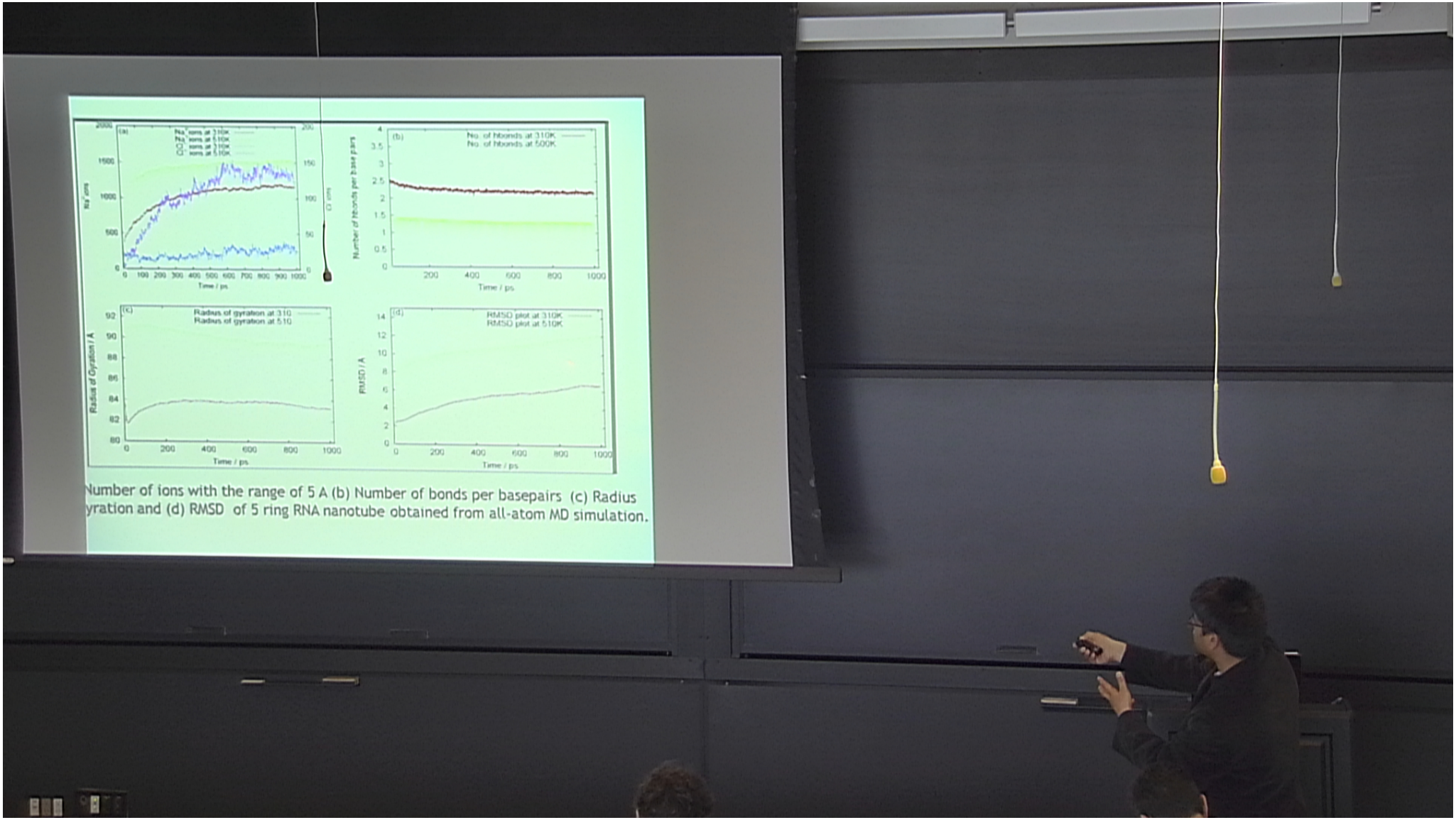
Number of Na^+ and Cl^- ions with the range of 5 A at 510K and the quenched run at 310K to see the evaporation of ions as temperature decreases.



Radial distribution function for the 5 ring RNA nanotube (a) P-P (b) P-OH2 (c) P-Na(d) P-Cl.

Conclusion…

- The all-atom MD simulations presented here are up to 1ns which is way below to the time taken in the biological processes. In view of this in mind we have developed the coarse-grained model of these systems which will allow us to perform MD simulation up to this time comparable to the real time used in biological process.



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