Educational Workshop Series

Five-Day Introductory Workshop on molecular modeling
Moleculoscope: Make them Dance, Make them Fold
(For 9th standard onwards)

Learn	How to use computers to solve problems in chemistry/physics/biology from a molecular perspective. We'll try to explore, understand and visualize nature through a molecular microscope: Moleculoscope! We'll learn how they interact, move, transform. We'll see how designing new molecules can improve the quality of our lives.
Organized by	• Exciting Science Group • Venture Center – a Technology Business Incubator
Co-sponsored by	DSM, Forbes Marshall Foundation, praj | foundation
Anchor Faculty	Dr. Suman Chakrabarty, NCL Pune
VC Organization Team	Shraddha Gargatti : Associate – Exciting Science Group Shiv Tripathi: Manager - ICT
For whom	• Children: Std 9 - 12 • Maximum 25 seats ➢ 20 seats (for those who bring their own laptops) ➢ 5 seats (reserved for children from municipal school) Booking schedule : **Free**; **First-come-first-serve**
When	• **Saturday, 7 June 2014-Thursday, 12 June 2014; 10 am-12:30pm**
Where	E Class Room, Venture Center, NCL Innovation Park Dr. Homi Bhabha (Pashan) Road, Pune-411008
Contact	**For registrations:** Ms Shraddha Gargatti Venture Center, 100, NCL Innovation Park, Dr. Homi Bhabha Road, Pune – 411008; Phone: +91-20-64011025 Email: outreach@excitingscience.org
Cost	• The workshop is free – however, CONFIRMED registration is mandatory. • Registration process: o Send email to outreach@excitingscience.org. Participants will be selected on a first-come-first-served basis. o Attend the Popular Talk on 18 May (Sunday, 10am) (visit www.excitingscience.org to register for the talk) o Bring a photocopy of your school ID card on the 18th May 2014 • Registration will be confirmed only if ALL the above steps are followed. • A final list of confirmed participants for the workshop will be available on the ESG website and participants will also be notified by email • Students will need to bring their own laptops (with install permissions) for the workshop

Why?

"Everything that living things do can be understood in terms of the jiggling and wiggling of atoms"

(Richard Feynman)

Course Outline

Computer simulation/Molecular modeling is emerging as a powerful tool in scientific research. This hands-on workshop intends to introduce school students to the power of computers in solving problems in physics/chemistry/biology. At the end of the workshop, students will have some familiarity with molecular modeling and will be able to perform elementary simulations at home.

We'll try to explore and visualize nature through a molecular microscope: we call this a **Moleculoscope**!

We'll learn why/how things happen the way they do around us. What determines if something is solid, liquid or gas? Why do oil and water not mix? How does salt dissolve in water? What are "proteins"? How do they work? Why do we get sick? How do the medicines work?

Can you design a new material, or new protein, or a new medicine? After all, they are nothing but molecules! ☺

Schedule

Time	Session title	Lead	Venue at Venture Center
7 June 2014	**Molecular view of Nature**		
9:30- 10:00 am	Registration	SG	Foyer Area
10:00-10:05 am	Introduction to the workshop and faculty	GK	E Classroom
10:05-11:15 am	**A molecular view of nature:** We'll look at some common natural phenomena through a molecular microscope (moleculoscope!) using computer modeling	SC	E Classroom
11:15-11:30am	**Break**		Foyer Area
11:30-12:30pm	Session continued	SC	E Classroom
9 June 2014	**Molecular Modeling**		
10:00-11:15am	**Basics of molecular modeling:** Types of molecular interactions, building simplified models, how to solve them using computers …	SC	E Classroom
11:15-11:30am	**Break**		Foyer Area
11:30-12:30pm	**Building the foundation:** basic thermodynamics, basic calculus, Newton's laws of motion, basic concepts of probability, basic programming	SC	E Classroom
10 June 2014	**Molecular Dynamics**		
10:00-11:15am	Your first **molecular dynamics** program! How to make the molecules move, heat them up, and watch the movie!	SC	E Classroom
11:15-11:30am	**Break**		Foyer Area
11:30-12:30pm	Session continued	SC	E Classroom
11 June 2014	**Proteins and Foldit**		
10:00-11:15 am	**Proteins: the molecular workhorses in our body** How do they work? What if they misbehave? How do the medicines work?	SC	E Classroom
11:15-11:30am	**Break**		Foyer Area
11:30-12:30pm	**Foldit:** Solve Puzzles for Science (https://fold.it/portal) A computer game for protein structure modeling/prediction: The higher you score, the better you fold!	SC	E Classroom
12 June 2014	**Foldit Challenges**		
10:00-11:15 am	Foldit challenges continued … (even when you leave the workshop)	SC	E Classroom
11:15-11:30am	**Break**		Foyer Area
11:30-12:30pm	Session continued	SC	E Classroom
12:30-1:00 pm	Distribution of certificates	GK	E Classroom

WORKSHOP FACULTY:

The workshop shall be run by Dr. Suman Chakrabarty, Ramanujan Fellow at CSIR-NCL, Pune

Education: Ph.D. (2010) in theoretical chemistry**:** Indian Institute of Science, Bangalore
Postdoctoral research: University of Southern California (USA); worked with a Nobel laureate!

Research Interests:
Using physics, mathematics, and computer programming to understand chemistry/biology.
Watching movies of molecules in action!
Designing new and useful molecules.

Other Interests:
Playing with computers and software (not just video games!)
Movies, music, books, photography, theater, travel …

Course includes

- Certificate of Participation issued by Exciting Science Group
- Workshop includes soft drink during the break at Foyer Area

About the Organizers	
	About Exciting Science Group The Exciting Science Group comprises of scientists from two of Pune's best research institutions, NCL and IISER-Pune. This initiative is aimed at conveying the excitement of science and technology to school students. The motivation behind our programme is to attract the brightest talent from the next generation towards careers in science and technology, since it will be these students who will drive tomorrow's science and innovation based economy. For more information, visit**:** **www.excitingscience.org**
	About Venture Center Entrepreneurship Development Center (Venture Center) – a CSIR initiative – is a Section 25 company hosted by the National Chemical Laboratory, Pune. Venture Center strives to nucleate and nurture technology and knowledge-based enterprises by leveraging the scientific and engineering competencies of the institutions in the Pune region in India. The Venture Center is a technology business incubator supported by the Department of Science & Technology's National Science & Technology Entrepreneurship Development Board (DST-NSTEDB). Venture Center's focuses on technology enterprises offering products and services exploiting scientific expertise in the areas of materials, chemicals and biological sciences & engineering. For more information, visit http://www.venturecenter.co.in/

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	About Forbes Marshall Foundation As an organization, Forbes Marshall has a long history of serving the communities it operates in; playing the role of a catalyst, enabling successful social change. Building on those experiences, the Forbes Marshall Foundation was set up, with the objective of supporting projects and communities, located outside of Pune, India. The Foundation's core principle is to "give" in a manner, which promotes sustainability of a project. The three core grant making priority areas are education, health - with a particular focus on neglected areas of health; and research, which would foster more enlightened and informed giving. For more information, visit: http://www.forbesmarshall.com/fm_micro/FMFoundation/
	About Praj Foundation Praj Foundation was established in 2004 to give expression to the sensitivities of Praj employees and family members towards societal responsibilities. While this was already happening in the Company, Praj Foundation helped put all its social impact activities under one roof with a clearly stated objective. The idea was to create areas of focus within the ambit of its social activities that would best reflect the strengths of the company. For more information, visit**:** http://www.praj.net/praj-foundation.html