

# MacDiarmid Access Grid Seminar

Thursday 3 September 12.15pm

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## Dmitri Schebarchov

School of Chemical and Physical Sciences, Victoria University of Wellington

“Mechanisms in carbon nanotube growth: a molecular dynamics study”

Even though Carbon Nanotubes (CNTs) are one of the most researched materials of the last two decades, their formation is still poorly understood. This restricts our ability to control the structure of CNTs during their growth, making it difficult to put their numerous potential applications into practice. In this talk I will present classical Molecular Dynamics simulations of three important issues in CNT synthesis, which is the focus of my PhD research. The melting transition in supported nanoparticles will be discussed first. The motivation behind this particular work is the ongoing debate of whether the catalyst is solid or liquid during CNT formation. Then I'll talk about capillary absorption of catalyst particles by CNTs. This issue not only has implications to CNT growth, but also has intriguing applications in nanofluidics and material science. Finally, I'll present our recent simulations of the cap-to-tube transition in the early stages of CNT formation.

and

## Srikanth Dhondi

School of Chemical and Physical Sciences, Victoria University of Wellington

“Coarse grained molecular dynamics simulations of polymers at nanoscale”

Studying the properties of polymers at nanoscale is important because of their potential applications in many nanodevices. Furthermore, the macromolecular nature of these materials can lead to interesting behavior when used in nanodevices. In this talk, I will first discuss molecular dynamics simulations of polymeric fluids in narrow channels and how patterned slip conditions can be exploited to enhance mixing. This has practical relevance directly in the area of micro/nano fluidics. Secondly, I will present a study of the capillary absorption of polymer droplets and discuss effect of chain length.

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## Venues

Victoria University of Wellington, Room RB 106

University of Canterbury, Level 1 Psychology Building

University of Otago, Teaching Facilities, Information Services Building

University of Auckland, 23 Symonds St, Rm 411, Chemistry Building 301



**The MacDiarmid Institute**

*for Advanced Materials and Nanotechnology*