Maria Stepanova, J Nanomedic Nanotechnol 3:1
doi: http://dx.doi.org/10.4172/2157-7439.S1.02

OMICS Group Conferences
Accelerating Scientific Discovery

International Conference and Exhibition on
Nanotechnology & Nanomedicine
March 12-14, 2012 Omaha Marriott, USA

TITLE

# Modeling of nanostructures: Nanocrystals, surfactants, and nano-biosystems

**Maria Stepanova**

National Institute for Nanotechnology NRC, Canada

Rational design and control of nanoscale objects and processes allow exploiting unique properties of matter that manifest at these dimensions. Development of computational platforms that would describe the hierarchical complexity of nanosystems is one of main objectives to address the nanotechnology challenge in the coming decade. This presentation demonstrates our broadly scoped numerical platform applied to understand and predict self-assembly of nanostructures. Since basic mechanisms of self-assembly are often fundamentally similar in different systems, a multidisciplinary approach is possible when a computational framework is applied to a broad variety of nanoscale self-assembly phenomena. The examples presented include our recent modeling of self-assembled synthesis of arrays of metallic nanocrystals, phase separation in surfactants, essential collective dynamics in biopolymers, and bioadsorption. The latter example includes a detailed modeling and numerical characterization of the interaction on an enzyme with a nanoparticle covered by a polymer brush. From these examples, it is shown how subtle interactions at the level of individual atoms or molecules may be implicated into processes occurring at higher system levels and bigger scales. Our modeling tools comprise molecular dynamics modeling, Langevin dynamics, kinetic Monte-Carlo simulations, and continuum kinetic modeling, including our original and unique methods. Applications to nanofabrication, biomembrane research, structural biology, and nanomedicine are addressed.

## Biography

Dr. Maria Stepanova is a Research Officer and Principal Investigator at the National Institute of Nanotechnology NRC (Alberta, Canada), and leads a broad multidisciplinary research on theory, modeling, and simulations of nanosystems. The multiscale numerical methodologies that Dr. Stepanova and her team employ comprise molecular dynamics, statistical mechanics, and kinetics frameworks. Dr. Stepanova and her team work to discover fundamental mechanisms that determine the complex structure and function of a broad variety of objects from nanocrystals to biopolymers, and develop novel and unique numerical tools to facilitate the design of nanoscale systems and processes. At NANO-2012, Dr. Stepanova presents her group's research and innovations in the areas of nanofabrication, structural biology, and nanomedicine.