University of Victoria | Graduate Studies

Notice of the Final Oral Examination
for the Degree of Master of Applied Science

of

PO ZHANG

BSc (University of Victoria, 2010)

"Electrical Properties of Metal-Molecular Nanoparticle Networks: Modeling and Experiment"

Department of Electrical and Computer Engineering

Thursday, August 25, 2016
10:00 A.M.
Engineering Office Wing
Room 230

Supervisory Committee:
Dr. Chris Papadopoulos, Department of Electrical and Computer Engineering, University of Victoria (Supervisor)
Dr. Mihai, Department of Electrical and Computer Engineering, UVic (Member)

External Examiner:
Dr. Dennis Hore, Department of Chemistry, UVic

Chair of Oral Examination:
Dr. Helen Kurki, Department of Anthropology, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

The electrical properties of metal-molecular nanoparticle networks are studied both theoretically and experimentally. Benzenedithiol-aluminum cluster linear chains, Y-shaped and H-shaped networks are modeled with semi-empirical methods to study the electronic properties of such structures. The HOMO (highest occupied molecular orbital)-LUMO (lowest unoccupied molecular orbital) gaps of the benzenedithiol-Al cluster networks decrease several eV compared to the isolated benzenedithiol molecule. Frontier energy levels become more closely spaced as the size of the molecular networks increase, accompanied with an increased HOMO energy and decreased LUMO energy, indicating a decreased energy barrier to electron transport. Delocalized spatial distribution of the frontier orbitals indicate a high probability for electron transmission and corresponds well with peaks near the HOMO-LUMO gap in the electronic density of states. Self-assembled molecular networks consisting of dithiol/thiol molecules and colloidal gold nanoparticles are fabricated with a solution-based method. Electrical measurements performed on these nanostructures show a typically linear current-voltage characteristic while nonlinear I-V curves are also observed for networks built of benzenedithiol or hexane/octanethiol molecules. Further analysis with atomic force microscopy shows that the network's conductance is determined by the molecule's conductivity and network dimensions. Circuit model consisting of networked molecular resistors is applied to study the interconnections between the particles within the network and the simulated values of the network's conductance is consistent with the measured values. Theoretical and experimental study on the electrical properties of metal-molecular nanoparticle networks reveals the influence of molecules and metallic particles on determining the network's conductivity. Such self-assembled networks can be used to implement several circuit elements, such as resistors, diodes, etc., and more complicated computation components such as nanocells, memristors, etc. The electrical properties of the networks can be tuned by proper choice of molecules, metallic particles and network geometry making them promising for molecular electronic circuits.