



**University
of Victoria**

Graduate Studies

Notice of the Final Oral Examination
for the Degree of Doctor of Philosophy

of

EMILIAN TUCA

MSc (Alexandru Ioan Cuza University, 2011)

BSc (Alexandru Ioan Cuza University, 2009)

**“Theoretical Investigations of Molecular Self-Assembly
on Symmetric Surfaces”**

Department of Chemistry

Friday, September 27, 2019

1:00 P.M.

Clearihue Building

Room B017

Supervisory Committee:

Dr. Irina Paci, Department of Chemistry, University of Victoria (Supervisor)

Dr. Cornelia Bohne, Department of Chemistry, UVic (Member)

Dr. Matthew Moffitt, Department of Chemistry, UVic (Member)

Dr. Byoung-Chul Choi, Department of Physics and Astronomy, UVic (Outside Member)

External Examiner:

Dr. Gren Patey, Department of Chemistry, University of British Columbia

Chair of Oral Examination:

Dr. Martin Farnham Department of Economics, UVic

Abstract

Surface self-assembly, the spontaneous aggregation of molecules into ordered, stable, noncovalently joined structures in the presence of a surface, is of great importance to the bottom-up manufacturing of materials with desired functionality. As a bulk phenomenon informed by molecular-level interactions, surface self-assembly involves coupled processes spanning multiple length scales. Consequently, a computational approach towards investigating surface self-assembled systems requires a combination of quantum-level electronic structure calculations and large-scale multi-body classical simulations. In this work we use a range of simulation approaches from quantumbased methods, to classical atomistic calculations, to mean-field approximations of bulk mixed phases, and explore the self-assembly strategies of simple dipoles and polyaromatic hydrocarbons on symmetric surfaces.