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

Dr. David Capson, Dean, Faculty of Graduate Studies
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.