THERMAL COUPLING AT AQUEOUS AND BIOMOLECULAR INTERFACES

by

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An Abstract of a Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the degree of

DOCTOR OF PHILOSOPHY

Major Subject: MATERIALS ENGINEERING

The original of the complete thesis is on file
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Troy, New York

May, 2010

ABSTRACT

Heat flow in the materials with nanoscopic features is dominated by thermal properties of the interfaces. While thermal properties of the solid-solid and solid-liquid interfaces are well studied, research of the thermal transport properties across soft (liquid-liquid) interfaces is very limited. Such interfaces are, however, plentiful in biological systems. In such systems the temperature control is of a great importance, because biochemical reactions, conformation of biomolecules as well as processes in biological cells and membranes have strong temperature sensitivity. The critical ingredient to temperature control in biological systems is the understanding of heat flow and thermal coupling across soft interfaces.

To investigate heat transfer across biological and aqueous interfaces we chose to study a number of soft interfacial systems by means of molecular dynamic simulations. One of the interfaces under our investigation is the interface between protein (specifically green fluorescent protein) and water. Using this model we concentrated on the importance of vibrational frequency on coupling between water and proteins, and on significant differences between the roles of low and high frequency vibrations. Our thermal interfacial analysis allowed us to shed new light on to the issue of protein to water slaving, i.e., the concept of water controlling protein dynamics.

Considering that the surface of the protein is composed of a complicated mixture of the hydrophobic and hydrophilic domains, to systematically explore the role of interfacial interactions we studied less complicated models with homogenous interfaces whith interfacial chemistry that could be changed in a controlled manner. We demonstrated that thermal transport measurements can be used to probe interfacial environments and to quantify interfacial bonding strength. Such ability provides a unique opportunity to characterize a variety of interfaces, which can be difficult to achieve with more direct structural characterization tools. We followed up with studies of models of heterogeneous interfaces where we addressed the issue of independent vs. correlated contributions of hydrophobic and hydrophilic interfacial regions to thermal transfer.

Finally we simulated heat flow across lipid bilayers which involve hydrophilic interfaces, but are characterized by relatively high surface roughness and non-saturated hydrocarbon chains. We found that roughness of the interface can significantly enhance thermal transport across the lipid membranes.