QUANTUM LOOP CURRENT IN MOLECULAR AND NANOSCALE JUNCTION DEVICES: THEORETICAL AND COMPUTATIONAL PERSPECTIVES

A Thesis Submitted

To

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Summary of the Thesis

This thesis deals with quantum loop current in molecular and nanoscale junction devices. The thesis is arranged into five chapters that collectively comprise the systematic study of the subject undertaken in this work. Each chapter begins with an abstract that provides the outline of the work and includes background information on the subject studied. Motivation leading to each work, as presented in Chapters 2 through 4, is described in the section, "Scope of the Work", followed by a discussion on the model and computational techniques employed in each work. The noteworthy findings of the study are presented in the "Results and Discussion" section. A summary and concluding remarks are included at the end of each of these chapters, followed by a list of relevant references from the past and present. Other related studies and results that are not included in the published papers are also presented. The last chapter offers a succinct assessment of the work covered in the thesis along with suggestions for further research on a few chosen topics.

Chapter 1 gives a brief review of the necessary background materials for the work carried out in this thesis starting with a preamble to the molecular electronics with a focus on single-molecule junction devices. The theoretical formulation of electron transport through a molecular junction based on Landauer's approach is presented. The description of the transmission function within Landauer's formulation and the non-equilibrium Green's function (NEGF)-based expression of current under the steady-state condition are presented. Various factors affecting the electron transport through the molecular junctions are discussed. The chapter concludes with an overview of molecular thermoelectricity, which also serves as a background for Chapter 4.

Chapter 2 focuses on the influence of magnetic field on electron transport through molecular quantum ring structure junctions and the associated effects. It is found that weak coupling is essential for the magnetic field-based current control in smaller structures, while its role is significantly less in larger structures. This observation is based on the tight-binding calculations of the electron transport through the polycyclic aromatic hydrocarbons (PAHs) of increasing size under the field application in the range, 0 to 10 Tesla. However, the increased magnetic flux

through larger structures enables the modulation of energy levels with relative ease, leading to current control at relatively small field values ($\sim$ few Tesla).

Chapter 3 discusses quantum loop current in an open ring system along with a method for calculating loop current (referred to herein as circular current) without determining the local currents. At the certian bias voltage range, the circular current at low coupling far exceeds the net current through the ring. The circular current-induced force in a ring junction is examined and the reliability issues concerning junction instability due to rupture of cavalent bonds in the ring owing to large induced force at resonant bias are explored.

Chapter 4 opens with a systematic investigation of thermoelectric properties of molecules in presence of a magnetic field. A benzene ring and C_{60} fullerene are considered for the purpose. The possibility of modulation of thermoelectric power by an applied magnetic field is explored.

Chapter 5 briefly summarizes the main conclusions of the work carried out in this thesis. The future direction of research in this area is discussed. A list of future works on a few selected topics is given, along with an outline and explanation.

The thesis concludes with the index of the thesis that fills the last pages.