DECLARATION

I declare that the thesis entitled "**Theoretical study of spin polarized electrical and thermal transport properties of mesoscopic systems**" has been prepared by me under the supervision of Prof. Anirban Misra, Department of Chemistry. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

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CERTIFICATE

This is to certify that **Mr. Sudip Sarkar** has prepared the thesis entitled **"Theoretical study of spin polarized electrical and thermal transport properties of mesoscopic systems"**, for the award of Doctorate of Philosophy in Chemistry degree of the University of North Bengal, under my supervision. He has carried out the work at Department of Chemistry, University of North Bengal. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

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PREFACE

In last few decades the nanomaterials are being continuously studied in the search for new spintronic and thermoelectric materials. The first chapter thereby provides a brief description about the progress in the field of spin polarized electrical conductivity along with thermoelectric properties of nanomaterials. Spin polarization is the origin of both spintronic property and magnetism in molecules and also in materials. Consequently the discussions on magnetism of materials along with spintronic property are included for the detailed account of spin polarization phenomenon. The methods to quantify the spintronic, magnetic thermoelectric properties are depicted in second chapter. Spin rich systems are the most suitable candidates as building blocks of spintronic materials and organic diradicals are inexpensive, easy to synthesize. In the third chapter the magnetism of diradicals studied by means of exchange coupling constant, which also quantifies the spin polarization present in the systems. Another well practiced method to generate spin polarization in a system is the doping or adsorption of magnetic adatoms in a non-magnetic material. Thus in the fourth chapter spintronic property of 3*d*-transition metal encapsulated C_{20} fullerenes is studied. In Chapter 5, the spin thermoelectric property of boron doped graphene nanoribbon is described. Spin dependent thermoelectric features also known as spin caloritronics is a new branch of spintronic, in which spin polarized electrical conductivity along with thermal conductivity is also studied. In the final chapter, the essence of all chapters and importance of the current study have been summarized.

List of Tables

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Published

1. Sarkar, S.; Goswami, T.; Bhattacharya, D.; Misra, A., On the performance of generalized valence bond theory in predicting magnetic exchange coupling constant in organic diradicals: A comparison with Hartree-Fock theory. *Comput. Theor. Chem.* **2017,** *1116*, 220-224.
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2. Participated on Frontiers in chemistry 2017-18, Organized by Department of Chemistry, University of North Bengal, Darjeeling.

3. Participated on International Year of the Periodic Table of Chemical Elements-2019, Organized by Department of Chemistry, University of North Bengal, Darjeeling.