Chapter 1

Spin polarization, electrical conductivity and thermal conductivity in nanomaterials

1.1 Introduction

The size effect of materials on electrical transport and thermal transport properties are being studied from the last century.[1-4] Primarily this domain of research area was focused on metals, semiconductors and electrolytes.[2,4,5, 6] However, in the recent time, scientists have shifted their focus on nanomaterials and nanoscale devices in this regime.[7, 8] Reduced dimension and size of such materials and their versatile applications in various fields including electronics and thermoelectric devices have been crafted them into a burning topic of research area. Nanoscale devices of organic molecules and nanomaterials are known to be very much useful in spintronics, memory devices and also in the field of quantum computing, due to their cheap cost, flexibility, reduced size and excellent electronic properties.[9-11]

1.2 Nanomaterials

Richard Feynman, the pioneer physicist has coined the idea of nanomaterials for the first time. Nanomaterials, often referred to as mesoscopic materials, are the class of materials, in which one or more physical dimensions remain constrained to the nanometer scale. Usually these materials exhibit physical properties in between the midway of purely quantum behavior of atoms and molecules and the classical behavior of bulk materials. The nanoscale size of such materials brings quantum confinement effect into them and subsequent increase in surface area and interfacial scattering of electron and phonon.[12-14] The reduced dimensionality and size affect the electronic properties and also their transport properties. Based on dimension and size several types of nanomaterials are known till date, e.g. nanosheet, nanotube, nanowire, nanobelt, nanoring etc. some of them are depicted in Fig. 1.1.

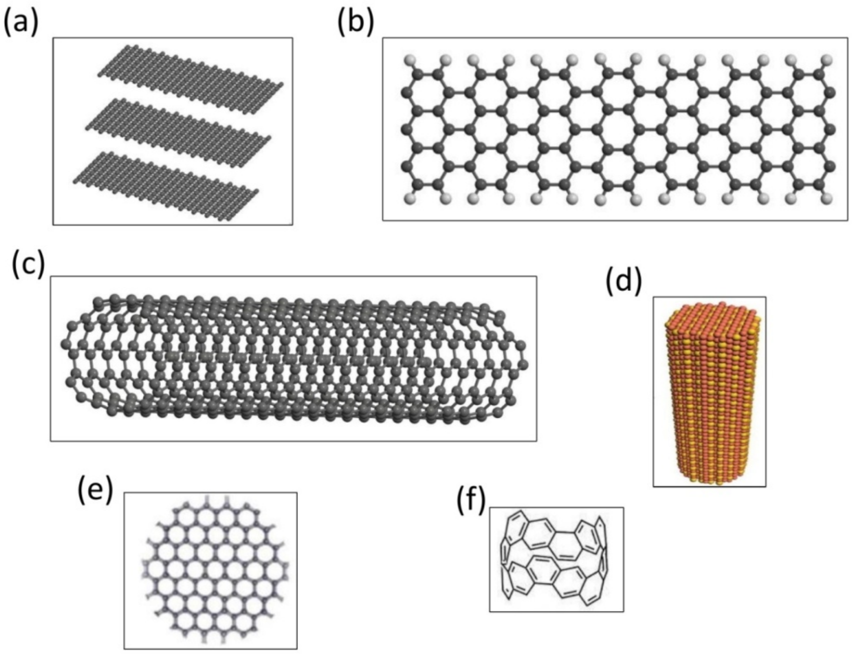

Figure 1.1 Various nanomaterials: (a) nanosheet, (b) nanoribbon, (c) nanotube, (d) nanoribbon, (e) quantum dot, (f) nanobelt.

1.3 Electrical transport properties of nanomaterials

Nanomaterials and nanoscale devices are of great interest as electrical parts of microchips, transistors, sensors and as building blocks of next generation electronics.[15, 16] On account of that, the study of transport properties of such materials particularly have drawn scientists' attention enormously. In this research area, carbon based nanomaterials like graphene, carbon nanotube and fullerene have been studied most widely.[17-20] Graphene is a two dimensional (2D) layer of one-atom-thick carbon atoms arranged in honeycomb lattices, has attracted attention of scientists and also known as wonder material due to its enormously high mechanical strength, large thermal conductivity and very high carrier mobility.[21-23] However, graphene is a semimetal with zero bandgap and several studies are carried out for the opening of the bandgap, among them patterning into nanoribons is the most popular.[22, 24, 25] Carbon nanotube is another class of carbon nonomaterials, which can be found in all metallic, halfmetallic and semiconductor.[26] Their band structure can be tuned with their chiral indices,[27] which characterizes their wrapping especially in single walled carbon nanotubes. The coherence length for spin propagation in CNTs is quite long (0.13–1.4 μm at 4.2 K),[28] because of very weak spin-orbit coupling and hyperfine interactions in carbon-based materials. That makes carbon nanotube an excellent candidate for quantum nanowire and spintronic applications.[29] Fullerenes are the zero dimensional carbon based nanomaterials, also studied exclusively for their exceptional transport properties.[30, 31] Fullerenes are cage like arrangement of carbon atoms that can incorporate metals endohedrally. Such endohedral metallofullerenes are being studied extensively as molecular swiching devices[32] and in quantum information processing.[33] Besides, carbon based nanomaterials, transition metal dichalcogenide (TMDC) such as MoS_2, $MoSe_2$, WS_2, WSe_2, *etc.*, are also studied for their application in nanoelectronics.[34-37] The 2D monolayers of TMDC have intrinsic bandgap of 1-4 ev, are often complement of graphene.[38] Nanoribnon and nanoclusters of TMDC also have been studied for their electronic, optical and magnetic properties.[38-41] All these studies sets up the stage for the present investigation.

1.3.1 Molecular electronics

With the growing interest of ever smallest possible electronics, transport property of devices made of molecules or materials like 2D monolayer sheet, 1D nanowire are investigated both theoretically and experimentally in last few decades.[18, 42-44] Such devices consist of molecule or nanomaterial placed between two electrodes (Fig. 1.2). These arrangements of electrode-molecule-electrode interface are known as nanoscale devices. When only charge transport of such devices is investigated for possible use of the molecule/material as electronics, this area of research is called molecular electronics. The study of spin transport along with charge is known as spintronics. Ratner *et. al.*, have discussed transport through a molecule theoretically for the first time and set a benchmark for molecular electronics.[45] Later, the discovery of STM devices and measurement of transport of molecules with it by several research groups have advanced the field of molecular electronics.[8, 46, 47] However, the techniques used for conductance measurement through a STM devices produce a large number of data set, because measurement can be made rapidly, which is the real problem faced by experimentalists.[48] To overcome this problem theoretical insight into the mechanism of transport becomes a necessity.

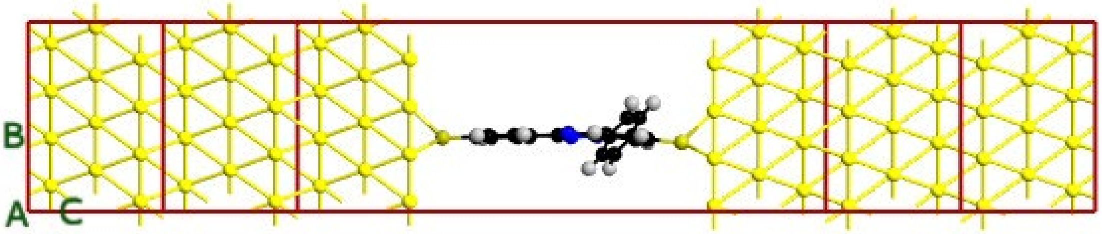

Figure 1.2 Schematic representation of molecular device for electronic transport calculation.

1.3.2 Molecular spintronics

Spintronics or spin based electronics is the combined study of both charge and spin transmissions through materials and devices. This field is an emerging branch of nanotechnology and is the combination of electronics and magnetism. This is currently one of the most attractive research areas within nanomagnetism, because it allows spin degree of freedom along with the charge within a material to process a signal of information.[49, 50] The key matter in this research area is the active manipulation of spin population near the Fermi level. The bands of electron which are responsible for conduction in a spintronic material, must be rich in spin density with respect to the either of spin, "majority spin" or "minority spin". The first significant study in this field is the finding of magnetoresistance in metallic multilayers by Fert *et. al*.[51] This discovery describes that the direction of carrier electrons could be controlled based on the spin magnetization of same electrons, and has opened up novel properties in materials for a completely new technology.

With the continuous developments in nanomaterials and nanotechnology and contemporary miniaturization of electronics to molecular scale has emerged a new field, namely molecular spintronics, which merges the unique properties of molecules to exhibit quantum effects and the concepts and ideas in spintronics, at the nanoscale.[52-54] This field has brought broad day-light on the organic semiconductors and organic molecules, which have extended π-network. Due to the weak spin-orbit and hyperfine coupling in these materials, spin relaxation time is longer than inorganic materials and on the other hand, flexibility and cheap cost make them ideal candidates for molecular spintronics.[55, 56] In this regard, the carbon nanotubes have been studied for long as spintronics materials, because of high spin coherence length over the 2D carbon network graphene.[29, 57] The organic radicals are also studied rigorously in this regime, due to the presence of unpaired electron in those systems.[58, 59]

1.3.3 Magnetism and spin polarization in molecular electronics

Spintronics and magnetism both are consequences of spin polarization in a system. Imbalance of up and down spin population of electrons in a system leads to spin polarization. Spintronic properties in a system could be achieved through several ways. One simple and probable way to serve this purpose is the injection of spin polarized charge carriers from a ferromagnetic electrode, which will act as a spin polarizer in the system.[60] Spin-polarization in nonmagnetic systems can also be induced by adsorbing magnetic adatoms, like atoms of transition metals and radicals.[61, 62] On the other hand, spintronic devices could be created from magnetic materials with intrinsic spin imbalance.[63] Although there are other possible ways to create spintronic characteristics, like modification of spin-orbit interactions, the above mentioned methods are studied widely and important progresses have been achieved.[64-66]

The magnetic materials are the prime focus for scientists to build a spintronic device, since inception.[67-69] In this context, inorganic complexes, nanosheets, nanowires, nanoclusters are investigated thoroughly for their excellent magnetic properties and hence spintronic behavior.[68-70] Consequently, various spintronic devices have been designed and fabricated successfully till date.[71-75] Alternately, the cheap cost, flexibility, weak spin orbit coupling and subsequent advances in the field of electronics, organic materials and molecules have attracted the attention of the scientists in this direction.[76-80] The challenge of making spintronic devices from non-magnetic organic systems have been overcome by adsorption of metals or magnetic adatoms on the surface or by doping.[81, 82] On the other hand, organic radicals have been frequently studied as spintronic devices for their intrinsic magnetism.[58]

1.3.4 Magnetism in organic radicals

From past few decades, scientists are looking for a new kind of magnetic material, where magnetism can be developed as one-molecule phenomenon rather than 3D magnetic ordering. This emerging field of material science has been known as molecular magnetism and probable applications of molecular magnets in the field of spintronic, superconductivity, photomagnetic switch etc., have attracted attention of experimentalists as well as theorists.[83-88] Among the precursors of molecular magnets stable organic radicals (Fig. 1.3), which could be synthesized and handled in pure state, are most suitable. The discovery of *β*-crystal phase *p*-nitrophenyl nitronyl nitroxide radical by Kinoswita *et. al.* has set a benchmark in this research area of molecular magnets and provide a thrust to the search for new ferromagnetic materials.[89] Nitronyl nitroxide diradicals with ethylene coupler shows a very high magnetic exchange coupling.[90] Another family of organic radicals is verdazyl radicals was first synthesized by Kuhn and Trischmann, are potential precursor for molecular magnets.[91-93]

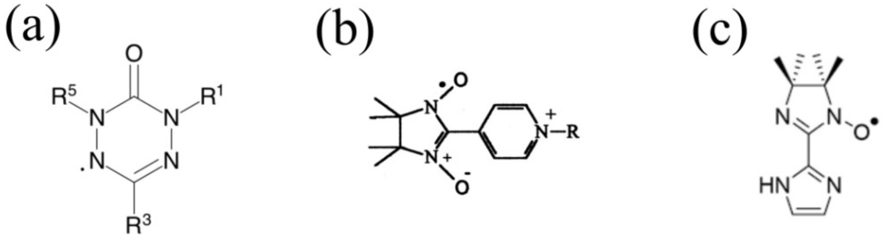

Figure. 1.3 Stable organic radicals: (a) oxoverdazyl, (b) nitronyl nitroxide, (c) imino nitroxide.

The interaction among the unpaired electrons is responsible for the excellent magnetic properties of organic radicals. The alignment of spins in organic radicals and their interaction through lone pairs or π electrons creates the residual spin magnetic moment in it. As a consequence, the design and synthesis of stable organic radicals with novel magnetic and electronic properties are essential for the development of spin science.

The electronic structure and magnetism of organic diradicals are often dependent on the couplers and can be modulated and organized for the intermolecular interaction of unpaired spins. Versatile applications of molecular magnets have led both theoretical design and synthesis of organic diradicals. Ziesel *et. al.* have studied and isolated diradicals of nitronyl nitroxide with ethylene coupler.[90] Turek and coworkers studied a series of iminonitroxide and nitronyl nitroxide diradical derivatives with phenylene and ethynylene coupler and shown that the spin polarization and molecular conformation controls the magnetism.[94] The study of non-kekule bis-oxoverdazyl diradical by Fico *et. al.* have found that the ground state of it is singlet with a little thermally populated triplet.[95] Gilroy and coworkers have synthesized derivatives of verdazyl radical and studied their magnetic properties.[96] Ali and Datta have studied bis-nitronyl nitroxide coupled with linear π-spacers and found that the magnetic interaction is transmitted through π-conjugation.[97] Ferromagnets based on oxoverdazyl and thiooxoverdazyl radicals with different polyacene couplers of varying length have studied by Bhattacharya *et. al.* and they found that the magnetic property strongly depends on the length of coupler and path of spin polarization.[98]

1.3.5 Electrical transport property of organic radicals

Organic radicals are intrinsic magnetic materials due to the presence of unpaired electrons in it. The spin polarization generated by the presence unequal spin population of electrons, long spin coherence length due to weak spin-orbit and hyperfine interaction make organic radicals ideal candidate for spintronic applications.[99] Hermann *et. al.* have studied the transport properties of simple π-type radicals placed between two gold electrodes and found that transmission does not directly depend on the MO occupations, because the population of spin up and down electrons influence the MO shapes and energies.[100] Wu and coworkers have theoretically investigated the transport properties of 1,3,5-triphenylverdazyl radical and spin Seebeck effect has been observed for the *p*-connection and 100% pure spin current for *m*-connection.[101] Bhattacharya *et. al.* have studied spin-polarized transport properties of *m*-phenylene connected bis-aminoxyl diradicals.[58]

1.3.6 Electrical transport properties of fullerenes

Fullerenes are bucky-ball shaped molecular allotropes of carbon which have attracted the attention of researchers and scientists, since the discovery of C_{60} fullerene in 1985 by Kroto *et. al.*[102] After that, lots of fullerenes of various sizes are discovered and studied (Fig. 1.4). In C_{60} fullerene all the carbon atoms are equivalent and sp^2 hybridized. It consists of 20 hexagons and 12 pentagons and is highly symmetrical with a high symmetry of icosahedra I_h. The cage like hollow structure of fullerene can accommodate atoms or small molecules inside it. Such doped fullerenes are termed as endohedral fullerenes and when metal atoms are encapsulated inside the carbon cage, are known as endohedral metallofullerenes (EMF).[103] Till date, a lots of endohedral fullerenes have been synthesized and studied both theoretically and experimentally, since those may break the "isolated pentagon rule" (IPR).[31, 104-108] This rule tells that the most stable geometry of a fullerene could be achieved by the formation of pentagons around the structure.

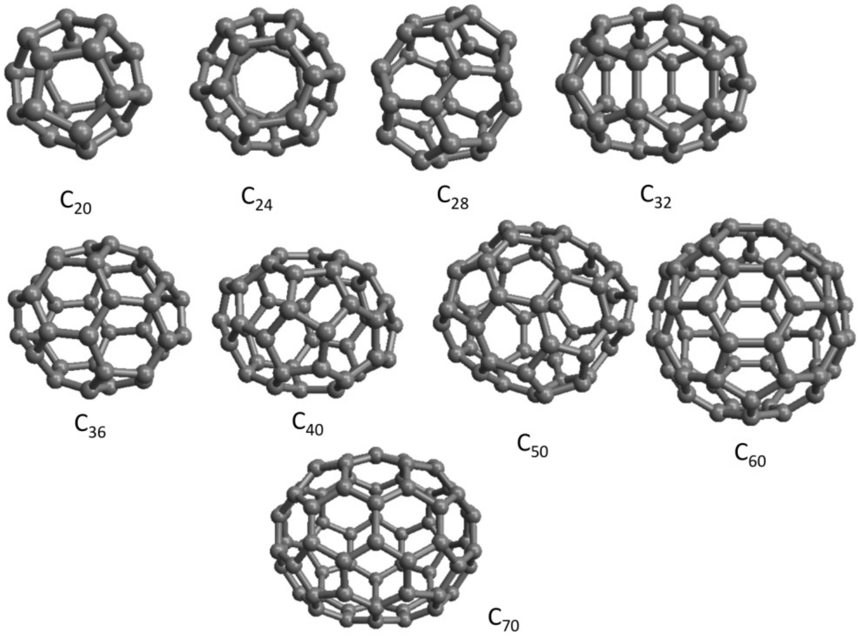

Figure 1.4 Fullerenes of different sizes.

Nowadays, small EMFs have attracted tremendous attention of the scientific community due to its excellent capacity as electron acceptor and ample applications in the field of photovoltaic materials, biomedical, electronic devices and so on.[104, 109-114] The ever smallest possible fullerene is C_{20}, which breaks the IPR as it consists of only pentagons.[115, 116] Among the all possible isomers of C_{20}, the most stable isomer is one with icosahedra I_h symmetry. The encapsulation of atoms including transition metals inside C_{20} has been studied by several research groups.[117, 118] Electrical transport properties of C_{20} fullerene and its derivatives were analyzed by many researchers.[119-121] Roland and coworkers have studied the transport properties of C_{20} fullerene chain and found that the conductance does not depend on the chain length.[120] Wang *et. al.* have investigated the negative differential resistance (NDR) effect of C_{20} fullerenes and found that it depends on the crystal field of gold electrode.[121] When C_{20} is placed between electrodes of Au(111) plane NDR vanishes. The insertion of magnetic adatoms, such as transition metals inside the C_{20} fullerene cage has been regularly exercised. Baei et. al. have studied transition metal encapsulated endohedral C_{20} metallofullerenes by first principle calculation.[117] Zhao and coworkers found that the Fe encapsulated C_{20} is the most stable among all 3*d*-transtion metal doped EMFs.[118] Such studies drive the application of C_{20} towards spintronics research. The spin dependent transport property of C_{20} and nitrogen encapsulated C_{20} EMF has been theoretically investigated.[122] This study is the first step towards the application of C_{20} as spintronic device.

1.4 Thermal conductivity of nanomaterials

Thermal conductivity is the study of heat transport through materials, carried by phonon and electrons. Generally in a bulk material, the 99% of heat is carried by phonons and the rest by electrons. As a consequence, to understand the thermal conductivity one must have proper knowledge of the spectrum of crystal vibration. As thermal conductivity is a property of crystal lattice, it does not only depend on the elements of the material, but also on the shape and size and temperature of the same.[123, 124] However, on reducing the dimension of a material, the thermal conductivity gets decreased. The thermal conductivity of a material also depends on the grain boundary of a material, on increasing the grain size it increases.[125]

The study of thermal transport has two aspects, firstly to get a material with high thermal conductivity, which can resolve the heat management issues in electronic industries by draining heat from electronic circuits. On the other hand, diminution of thermal conductivity in a thermoelectric material enhances its efficiency. Thermoelectric materials can convert heat into electricity by means of Seebeck effect, which have attracted the attention of scientific community and researchers for its practical utility. The nanomaterials are more useful in such thermoelectric application, as the low dimension materials have lesser thermal conductivity compared to bulk counterpart. Nevertheless, the modern era of electronic industry is getting shifted towards nanomaterials by miniaturization of electronic circuits. So, to fulfill both the aspects of thermal transport phenomena mentioned above, theoretical and experimental investigations of thermal transport properties of nanomaterials are essential.

1.4.1 Thermoelectric figure of merit (ZT)

The thermoelectric figure of merit is the coefficient of a system, which determines the efficiency to convert heat into electricity and vice versa, defined as $ZT = \frac{S^2\sigma T}{K}$, where S is the Seebeck coefficient, σ is electrical conductivity, K is thermal conductivity and T is the temperature. This coefficient is a unitless quantity, which is linearly proportional with electrical conductivity of a material, whereas inversely proportional with the thermal conductivity. Due to this reason, to get a significant thermoelectric figure of merit (≈ 3) in a system, high electrical conductivity along with low thermal conductivity is mandatory and also a high Seebeck coefficient. However, to meet all these requirements simultaneously for high ZT is a challenging task, because the materials with high electrical conductivity generally have high thermal conductivity and a low Seebeck coefficient. As a consequence transition metals, materials of main group elements are not good thermoelectric materials. Continuous search for thermoelectric materials with high ZT have found lots of efficient thermoelectric materials, like Bi_2Se_3, Bi_2Te_3, SiGe, SnSe, PbTe, BiSbTe, Cu_2Se, Cu_2S, $CuInSe_2$, $Mg_3(Bi,Sb)_2$ and so on.[126-134] However, these materials are limited to practical applications due to less abundance, toxicity, instability at high temperature and cost ineffectiveness. Nevertheless, there are many ways to overcome this problem among them one of the best possible strategy is to find new materials of main group element with high ZT. To serve this purpose organic materials are the most suitable due to their low cost, stability at high temperature, natural abundance and easy handling. In this regard lots of organic thermoelectric materials with moderate ZT have been discovered and studied. But organic thermoelectric materials with high ZT are yet to be discovered. Another possible strategy to overcome the above mentioned problem is to use the thermoelectric materials with moderate ZT in a smart way, in which the thermal current can be converted to spin current.[135, 136] Such materials are termed as spin thermoelectric materials.[137-141]

1.4.2 Spin thermoelectric figure of merit

Spin thermoelectrics is a new branch of spintronics and thermoelectrics, in which the spin degree of freedom is added to the thermoelectric materials. The discovery of spin thermolelectric materials can be traced back to the work done by Uchida *et. al.*, describes the conversion of thermal current to spin electricity for the first time in a $Fe_{81}Ni_{19}$ thin film.[142] This phenomenon of conversion thermal current to spin current is known as spin dependent Seebeck effect (SDSE), whereas, when ferromagnetic electrodes are attached with non magnetic material as spin injector, this phenomenon is known as spin Seebeck effect (SSE).[127, 135, 136] SDSE can occur in bulk ferromagnets, which is a direct consequence of unequal spin up and down currents generated due to spin polarization.[136] Whereas, SSE occurs in two steps, in the first step a spin current is generated from thermal current in the ferromagnetic electrodes and second step is the injection of the spin current to the non-magnetic conductor across the interface.[136, 143] To serve the purpose, semiconductors of transition metal with intrinsic spin polarization are the best candidates. Spin thermoelectric feature of lots of transition metal semiconductors have been successfully synthesized and investigated both theoretically and experimentally.[137, 140-142, 144] However, short spin coherence length due to strong spin-orbit coupling, cost ineffectiveness, instability at high temperature these materials do not have significant usefulness. Whereas, the weak spin-orbit coupling, lower cost, flexibility in synthesis of organic materials make them more suitable candidates for SSE. Till date so many organic organic materials are studied for spin thermoelectric features and synthesized, still more effort should be provided in this regard.[145-147]

1.4.3 Spin thermoelectric properties of graphene nanoribbons

The wonder material graphene is the most studied nanomaterial in last two decades.[148-152] The Seebeck coefficient of graphene is high compared to the other nanomaterials, but due to high thermal conductivity the *ZT* is negligible and it is not a thermoelectric material.[153] When graphene is patterned into a nanoribbon, a direct bandgap appears depending on the width of the nanoribbon.[154] The low thermal conductivity in semiconductor graphene nanoribbons (GNRs) and high Seebeck coefficient due to direct bandgap make it suitable candidate for thermoelectric application.[155-158] GNRs are broadly divided into two categories by their edge characteristics, namely, armchair GNRs (AGNRs) and zigzag GNRs (ZGNRs) (Fig. 1.5). AGNRs are non-magnetic semiconductor, whereas, the ground state of ZGNRs is antiferromagnetic with a net zero spin.[159, 160] So, ZGNRs are more suitable GNRs for spintronic and hence spin-thermoelectric application. But the zigzag edges of GNRs are very much unstable, due to which synthesis of ZGNRs is very difficult.[161] Whereas, a lots of bottom-up approach for the synthesis of AGNRs are already been reported.[162-164] The spin-thermoelectric features of ZGNRs have been studied in presence of magnetic field and ferromagnetic electrodes.[146, 147, 165, 166] In a recent work, Sierra *et. al.* have frabricated a spin caloritronic device based on graphene and ferromagnetic electrodes and generated spin current from thermal gradient.[145] Chico and workers have studied spin and charge component of two overlapping AGNRs in presence ferromagnetic electrodes.[167]

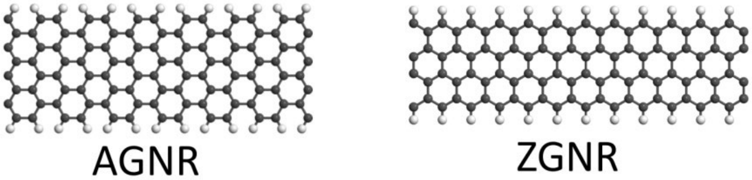

Figure 1.5 Various graphene nanoribbons.

Farghadan *et. al.* have studied spin and charge thermoelectric features of a device made of AGNRs and ZGNRs scattering region and effects of antidots on *ZT* have been considered.[168]

1.5 Objectives of the thesis

The objectives of the current thesis are to theoretically study the spin polarized electrical transport property and thermal transport property of nanomaterials. The defined objectives of the thesis are as follow:

(1) To investigate the spin polarization in organic diradicals estimated by exchange coupling constant (Chapter 3; On the performance of generalized valence bond theory in predicting magnetic exchange coupling constant in organic diradicals).

(2) To theoretically study the spin-polarized transport property of C_{20} metallofullerenes by inserting 3d-transition metals (Chapter 4; Spin-polarized electrical transport in transition metal encapsulated C_{20} fullerenes).

(3) To calculate the spin-thermoelectric figure of merit along with tunneling magnetoresistance of boron doped graphene nanoribbon (Chapter 5; Spin-thermoelectric properties and giant tunneling magnetoresistance of boron-substituted graphene nanoribbon).

1.6 References

1. Friedman, A. N., Some effects of sample size on electrical transport in Bismuth. *Phys. Rev.* **1967**, *159* (3), 553.

2. Macdonald, D. K. C.; Sarginson, K., Size effect variation of the electrical conductivity of metals. *Proc. R. Soc. A: Math. Phys. Eng. Sci.* **1950**, *203* (1073), 223-240.

3. Nath, P.; Chopra, K., Thermal conductivity of copper films. *Thin Solid Films* **1974**, *20* (1), 53-62.

4. Issi, J.-P.; Mangez, J., Size dependence of the transport properties of bismuth in the phonon-drag region. *Phys. Rev. B* **1972**, *6* (12), 4429.

5. Mott, N. F., The electrical conductivity of transition metals. *Proc. R. Soc. A: Math. Phys. Eng. Sci.* **1936**, *153* (880), 699-717.

6. Bronstein, H.; Bredig, M., The electrical conductivity of solutions of alkali metals in their molten halides1. *J. Am. Chem. Soc.* **1958**, *80* (9), 2077-2081.

7. Joachim, C.; Ratner, M. A., Molecular electronics. *Proc. Natl. Acad. Sci.* **2005**, *102* (25), 8800-8800.

8. Tao, N. J., Electron transport in molecular junctions. *Nat. Nanotechnol.* **2010**, 185-193.

9. Bogani, L.; Wernsdorfer, W., Molecular spintronics using single-molecule magnets. *Nat. Nanotechnol.* **2010**, 194-201.

10. Wang, K.; Alzate, J.; Amiri, P. K., Low-power non-volatile spintronic memory: STT-RAM and beyond. *J. Phys. D: Appl. Phys.* **2013**, *46* (7),074003.

11. Engel, H.-A.; Recher, P.; Loss, D., Electron spins in quantum dots for spintronics and quantum computation. *Solid State Commun.* **2001**, *119* (4-5), 229-236.

12. Hochbaum, A. I.; Chen, R.; Delgado, R. D.; Liang, W.; Garnett, E. C.; Najarian, M.; Majumdar, A.; Yang, P., Enhanced thermoelectric performance of rough silicon nanowires. *Nature* **2008**, *451* (7175), 163-167.

13. Boukai, A. I.; Bunimovich, Y.; Tahir-Kheli, J.; Yu, J.-K.; Goddard Iii, W. A.; Heath, J. R., Silicon nanowires as efficient thermoelectric materials. *Nature* **2008**, *451* (7175), 168-171.

14. Markussen, T., Surface disordered Ge–Si core–shell nanowires as efficient thermoelectric materials. *Nano Lett.* **2012**, *12* (9), 4698-4704.

15. Rojo, M. M.; Calero, O. C.; Lopeandia, A.; Rodriguez-Viejo, J.; Martin-Gonzalez, M., Review on measurement techniques of transport properties of nanowires. *Nanoscale* **2013**, *5* (23), 11526-11544.

16. Dai, H.; Wong, E. W.; Lieber, C. M., Probing electrical transport in nanomaterials: conductivity of individual carbon nanotubes. *Science* **1996**, *272* (5261), 523-526.

17. Yang, Y.; Brenner, K.; Murali, R., The influence of atmosphere on electrical transport in graphene. *Carbon* **2012**, *50* (5), 1727-1733.

18. Ma, T.; Liu, Z.; Wen, J.; Gao, Y.; Ren, X.; Chen, H.; Jin, C.; Ma, X.-L.; Xu, N.; Cheng, H.-M., Tailoring the thermal and electrical transport properties of graphene films by grain size engineering. *Nat. Commun.* **2017**, *8* (1), 1-9.

19. Eletskii, A. V., Transport properties of carbon nanotubes. *Phys.-Uspekhi* **2009**, *52* (3), 209.

20. Shimada, T.; Ohno, Y.; Okazaki, T.; Sugai, T.; Suenaga, K.; Kishimoto, S.; Mizutani, T.; Inoue, T.; Taniguchi, R.; Fukui, N., Transport properties of C_{78}, C_{90} and $Dy@C_{82}$ fullerenes-nanopeapods by field effect transistors. *Physica E Low Dimens. Syst. Nanostruct.* **2004**, *21* (2-4), 1089-1092.

21. Geim, A. K., Graphene: status and prospects. *Science* **2009**, *324* (5934), 1530-1534.

22. Novoselov, K. S.; Fal, V.; Colombo, L.; Gellert, P.; Schwab, M.; Kim, K., A roadmap for graphene. *Nature* **2012**, *490* (7419), 192-200.

23. Ren, W.; Cheng, H.-M., The global growth of graphene. *Nat. Nanotechnol.* **2014**, *9* (10), 726-730.

24. Lu, G.; Yu, K.; Wen, Z.; Chen, J., Semiconducting graphene: converting graphene from semimetal to semiconductor. *Nanoscale* **2013**, *5* (4), 1353-1368.

25. Wilhelm, J.; Walz, M.; Evers, F., Ab initio quantum transport through armchair graphene nanoribbons: Streamlines in the current density. *Phys. Rev. B* **2014**, *89* (19), 195406.

26. Laird, E. A.; Kuemmeth, F.; Steele, G. A.; Grove-Rasmussen, K.; Nygård, J.; Flensberg, K.; Kouwenhoven, L. P., Quantum transport in carbon nanotubes. *Rev. Mod. Phys.* **2015**, *87* (3), 703.

27. Dresselhaus, G.; Dresselhaus, M. S.; Saito, R., *Physical properties of carbon nanotubes*. World scientific, 1998.

28. Tsukagoshi, K.; Alphenaar, B. W.; Ago, H., Coherent transport of electron spin in a ferromagnetically contacted carbon nanotube. *Nature* **1999**, *401* (6753), 572-574.

29. Kuemmeth, F.; Churchill, H. O. H.; Herring, P. K.; Marcus, C. M., Carbon nanotubes for coherent spintronics. *Mater. Today.* **2010**, *13* (3), 18-26.

30. Wang, F.; Li, G., Electron transport properties and spin modulation effect analysis for C 60, Au@C_{60} and Ag@C_{60}. *Appl. Phys. A* **2016**, *122* (4), 366.

31. Kareev, I.; Bubnov, V.; Laukhina, E.; Koltover, V.; Yagubskii, E., Endohedral metallofullerenes M@C_{82} (M= La, Y): synthesis and transport properties. *Carbon* **2003**, *41* (7), 1375-1380.

32. Yasutake, Y.; Shi, Z.; Okazaki, T.; Shinohara, H.; Majima, Y., Single molecular orientation switching of an endohedral metallofullerene. *Nano Lett.* **2005**, *5* (6), 1057-1060.

33. Harneit, W., Fullerene-based electron-spin quantum computer. *Phys. Rev. A* **2002**, *65* (3), 032322.

34. Schmidt, H.; Wang, S.; Chu, L.; Toh, M.; Kumar, R.; Zhao, W.; Castro Neto, A.; Martin, J.; Adam, S.; Özyilmaz, B., Transport properties of monolayer MoS2 grown by chemical vapor deposition. *Nano Lett.* **2014**, *14* (4), 1909-1913.

35. Huang, C.; Wu, S.; Sanchez, A. M.; Peters, J. J.; Beanland, R.; Ross, J. S.; Rivera, P.; Yao, W.; Cobden, D. H.; Xu, X., Lateral heterojunctions within monolayer $MoSe_2$–WSe_2 semiconductors. *Nat. Mater.* **2014**, *13* (12), 1096-1101.

36. Ovchinnikov, D.; Allain, A.; Huang, Y.-S.; Dumcenco, D.; Kis, A., Electrical transport properties of single-layer WS_2. *ACS nano* **2014**, *8* (8), 8174-8181.

37. Zhou, H.; Wang, C.; Shaw, J. C.; Cheng, R.; Chen, Y.; Huang, X.; Liu, Y.; Weiss, N. O.; Lin, Z.; Huang, Y., Large area growth and electrical properties of p-type WSe_2 atomic layers. *Nano Lett.* **2015**, *15* (1), 709-713.

38. Sorkin, V.; Pan, H.; Shi, H.; Quek, S.; Zhang, Y., Nanoscale transition metal dichalcogenides: structures, properties, and applications. *Crit. Rev. Solid State Mater. Sci* **2014**, *39* (5), 319-367.

39. Hashemi, Z.; Rafiezadeh, S.; Hafizi, R.; Hashemifar, S. J.; Akbarzadeh, H., First-principles study of MoS_2 and $MoSe_2$ nanoclusters in the framework of evolutionary algorithm and density functional theory. *Chem. Phys. Lett.* **2018**, *698*, 41-50.

40. Li, T.; Galli, G., Electronic properties of MoS_2 nanoparticles. *J. Phys. Chem. C* **2007**, *111* (44), 16192-16196.

41. Wilcoxon, J.; Newcomer, P.; Samara, G., Synthesis and optical properties of MoS_2 and isomorphous nanoclusters in the quantum confinement regime. *J. Appl. Phys.* **1997**, *81* (12), 7934-7944.

42. Peng, L.; Yao, K.; Zhu, S.; Ni, Y.; Zu, F.; Wang, S.; Guo, B.; Tian, Y., Spin transport properties of partially edge-hydrogenated MoS_2 nanoribbon heterostructure. *J. Appl. Phys.* **2014**, *115* (22), 223705.

43. Bloom, F.; Wagemans, W.; Kemerink, M.; Koopmans, B., Separating positive and negative magnetoresistance in organic semiconductor devices. *Phys. Rev. Lett.* **2007**, *99* (25), 257201.

44. Bhowmick, R.; Koley, S.; Chattopadhyaya, M.; Sen, S., *g*–C_4N_3–graphene-*g*- C_4N_3: A useful spin thermoelectric material. *J. Phys. Chem. Solids.* **2021**, *156*, 110186.

45. Aviram, A.; Ratner, M. A., Molecular rectifiers. *Chem. Phys. Lett.* **1974**, *29* (2), 277-283.

46. Reed, M. A.; Zhou, C.; Muller, C.; Burgin, T.; Tour, J., Conductance of a molecular junction. *Science* **1997**, *278* (5336), 252-254.

47. Venkataraman, L.; Klare, J. E.; Nuckolls, C.; Hybertsen, M. S.; Steigerwald, M. L., Dependence of single-molecule junction conductance on molecular conformation. *Nature* **2006**, *442* (7105), 904-907.

48. Ratner, M., A brief history of molecular electronics. *Nat. Nanotechnol.* **2013**, *8* (6), 378-381.

49. Pulizzi, F., Spintronics. *Nat. Mater.* **2012**, *11* (5), 367-367.

50. Dietl, T.; Awschalom, D. D.; Kaminska, M.; Ohno, H., *Spintronics*. Academic Press: 2009.

51. Fert, A.; Grünberg, P.; Barthélémy, A.; Petroff, F.; Zinn, W., Layered magnetic structures: interlayer exchange coupling and giant magnetoresistance. *J. Magn. Magn. Mater.* **1995**, *140*, 1-8.

52. Awschalom, D. D.; Flatté, M. E., Challenges for semiconductor spintronics. *Nat. Phys.* **2007**, *3* (3), 153-159.

53. Dery, H.; Dalal, P.; Sham, L., Spin-based logic in semiconductors for reconfigurable large-scale circuits. *Nature* **2007**, *447* (7144), 573-576.

54. Xiong, Z.; Wu, D.; Vardeny, Z. V.; Shi, J., Giant magnetoresistance in organic spin-valves. *Nature* **2004**, *427* (6977), 821-824.

55. Alam, K. M.; Singh, A. P.; Starko-Bowes, R.; Bodepudi, S. C.; Pramanik, S., Template-assisted synthesis of π-conjugated molecular organic nanowires in the sub-100 nm regime and device implications. *Adv. Funct. Mater.* **2012**, *22* (15), 3298-3306.

56. Avdoshenko, S. M.; Ioffe, I. N.; Cuniberti, G.; Dunsch, L.; Popov, A. A., Organometallic complexes of graphene: toward atomic spintronics using a graphene web. *ACS nano* **2011**, *5* (12), 9939-9949.

57. Hueso, L. E.; Pruneda, J. M.; Ferrari, V.; Burnell, G.; Valdes-Herrera, J. P.; Simons, B. D.; Littlewood, P. B.; Artacho, E.; Fert, A.; Mathur, N. D., Transformation of spin information into large electrical signals using carbon nanotubes. *Nature* **2007**, *445* (7126), 410-413.

58. Shil, S.; Bhattacharya, D.; Misra, A.; Klein, D. J., A high-spin organic diradical as a spin filter. *Phys. Chem. Chem. Phys.* **2015**, *17* (36), 23378-23383.

59. Ratera, I.; Veciana, J., Playing with organic radicals as building blocks for functional molecular materials. *Chem. Soc. Rev.* **2012**, *41* (1), 303-349.

60. Zhu, H.; Ramsteiner, M.; Kostial, H.; Wassermeier, M.; Schönherr, H.-P.; Ploog, K., Room-temperature spin injection from Fe into GaAs. *Phys. Rev. Lett.* **2001**, *87* (1), 016601.

61. Johll, H.; Lee, M. D. K.; Ng, S. P. N.; Kang, H. C.; Tok, E. S., Influence of interconfigurational electronic states on Fe, Co, Ni-silicene materials selection for spintronics. *Sci. Rep.* **2014**, *4* (1), 1-7.

62. Ding, Y.; Wang, Y., Structural, electronic, and magnetic properties of adatom adsorptions on black and blue phosphorene: a first-principles study. *J. Phys. Chem. C* **2015**, *119* (19), 10610-10622.

63. Wu, P.; Yin, N.; Li, P.; Cheng, W.; Huang, M., The adsorption and diffusion behavior of noble metal adatoms (Pd, Pt, Cu, Ag and Au) on a MoS_2 monolayer: a first-principles study. *Phys. Chem. Chem. Phys.* **2017**, *19* (31), 20713-20722.

64. Shick, A. B.; Khmelevskyi, S.; Mryasov, O. N.; Wunderlich, J.; Jungwirth, T., Spin-orbit coupling induced anisotropy effects in bimetallic antiferromagnets: A route towards antiferromagnetic spintronics. *Phys. Rev. B* **2010**, *81* (21), 212409.

65. Covaci, L.; Berciu, M., Polaron formation in the presence of Rashba spin-orbit coupling: implications for spintronics. *Phys. Rev. Lett.* **2009**, *102* (18), 186403.

66. Caetano, R., Spin-current and spin-splitting in helicoidal molecules due to spin-orbit coupling. *Sci. Rep.* **2016**, *6* (1), 1-11.

67. Chen, W.; Godlewski, M.; Ruterana, P., Dilute Magnetic Materials for Spintronic Applications. *Phys. Status Solidi A* **2007**, *204* (1), 13-13.

68. Liu, J. P.; Fullerton, E.; Gutfleisch, O.; Sellmyer, D. J., *Nanoscale magnetic materials and applications*. Springer: 2009.

69. Haq, B. U.; Ahmed, R.; Shaari, A.; Afaq, A.; Tahir, B.; Khenata, R., First-principles investigations of Mn doped zinc-blende ZnO based magnetic semiconductors: Materials for spintronic applications. *Mater. Sci. Semicond. Process.* **2015**, *29*, 256-261.

70. Droghetti, A.; Baadji, N.; Sanvito, S., MgN: A possible material for spintronic applications. *Phys. Rev. B* **2009**, *80* (23), 235310.

71. Majumdar, S.; Laiho, R.; Laukkanen, P.; Väyrynen, I.; Majumdar, H. S.; Österbacka, R., Application of regioregular polythiophene in spintronic devices: Effect of interface. *Appl. Phys. Lett.* **2006**, *89* (12), 122114.

72. Fan, D.; Angizi, S.; He, Z. In *In-memory computing with spintronic devices*, 2017 IEEE Computer Society Annual Symposium on VLSI (ISVLSI), IEEE, 2017; pp 683-688.

73. Androulakis, J.; Gardelis, S.; Giapintzakis, J.; Gagaoudakis, E.; Kiriakidis, G., Indium oxide as a possible tunnel barrier in spintronic devices. *Thin Solid Films* **2005**, *471* (1-2), 293-297.

74. Zhang, D.; Zeng, L.; Cao, K.; Wang, M.; Peng, S.; Zhang, Y.; Zhang, Y.; Klein, J.-O.; Wang, Y.; Zhao, W., All spin artificial neural networks based on compound spintronic synapse and neuron. *IEEE Trans. Biomed. Circuits Syst.* **2016**, *10* (4), 828-836.

75. Chen, Y.; Zhou, Y.; Wang, L.; Cui, Z.; Huq, E.; Pan, G., Nanofabrication of spintronic devices with ultra small ferromagnetic contacts. *Microelectron. Eng.* **2008**, *85* (5-6), 1152-1156.

76. Naber, W.; Faez, S.; van der Wiel, W. G., Organic spintronics. *J. Phys. D: Appl. Phys.* **2007**, *40* (12), R205.

77. Boehme, C.; Lupton, J. M., Challenges for organic spintronics. *Nat. Nanotechnol.* **2013**, *8* (9), 612-615.

78. Bergenti, I.; Dediu, V.; Prezioso, M.; Riminucci, A., Organic spintronics. *Philos. Trans. Royal Soc. A* **2011**, *369* (1948), 3054-3068.

79. Morley, N.; Rao, A.; Dhandapani, D.; Gibbs, M.; Grell, M.; Richardson, T., Room temperature organic spintronics. *J. Appl. Phys.* **2008**, *103* (7), 07F306.

80. Lupton, J. M.; McCamey, D. R.; Boehme, C., Coherent spin manipulation in molecular semiconductors: getting a handle on organic spintronics. *ChemPhysChem* **2010**, *11* (14), 3040-3058.

81. Iancu, V.; Braun, K.-F.; Schouteden, K.; Van Haesendonck, C., Inducing magnetism in pure organic molecules by single magnetic atom doping. *Phys. Rev. Lett.* **2014**, *113* (10), 106102.

82. Nair, R.; Tsai, I.-L.; Sepioni, M.; Lehtinen, O.; Keinonen, J.; Krasheninnikov, A.; Neto, A. C.; Katsnelson, M.; Geim, A.; Grigorieva, I., Dual origin of defect magnetism in graphene and its reversible switching by molecular doping. *Nat. Commun.* **2013**, *4* (1),1-6.

83. Matsuda, K.; Matsuo, M.; Irie, M., Photoswitching of intramolecular magnetic interaction using diarylethene with oligothiophene π-conjugated chain. *J. Org. Chem.* **2001**, *66* (26), 8799-8803.

84. Tanifuji, N.; Irie, M.; Matsuda, K., New photoswitching unit for magnetic interaction: diarylethene with 2, 5-bis (arylethynyl)-3-thienyl group. *J. Am. Chem. Soc.* **2005**, *127* (38), 13344-13353.

85. Kobayashi, H.; Kobayashi, A.; Cassoux, P., BETS as a source of molecular magnetic superconductors (BETS= bis (ethylenedithio) tetraselenafulvalene). *Chem. Soc. Rev.* **2000**, *29* (5), 325-333.

86. Uji, S.; Shinagawa, H.; Terashima, T.; Yakabe, T.; Terai, Y.; Tokumoto, M.; Kobayashi, A.; Tanaka, H.; Kobayashi, H., Magnetic-field-induced superconductivity in a two-dimensional organic conductor. *Nature* **2001**, *410* (6831), 908-910.

87. Prinz, G. A., Magnetoelectronics. *Science* **1998**, *282* (5394), 1660-1663.

88. Emberly, E. G.; Kirczenow, G., Molecular spintronics: spin-dependent electron transport in molecular wires. *Chem. Phys.* **2002**, *281* (2-3), 311-324.

89. Tamura, M.; Nakazawa, Y.; Shiomi, D.; Nozawa, K.; Hosokoshi, Y.; Ishikawa, M.; Takahashi, M.; Kinoshita, M., Bulk ferromagnetism in the β-phase crystal of the p-nitrophenyl nitronyl nitroxide radical. *Chem. Phys. Lett.* **1991**, *186* (4-5), 401-404.

90. Ziessel, R.; Stroh, C.; Heise, H.; Köhler, F. H.; Turek, P.; Claiser, N.; Souhassou, M.; Lecomte, C., Strong exchange interactions between two radicals attached to nonaromatic spacers deduced from magnetic, EPR, NMR, and electron density measurements. *J. Am. Chem. Soc.* **2004**, *126* (39), 12604-12613.

91. Kuhn, R.; Trischmann, H., Surprisingly stable nitrogenous free radicals. *Angew. Chem. Int. Ed.* **1963**, *2* (3), 155-155.

92. Takeda, K.; Hamano, T.; Kawae, T.; Hidaka, M.; Takahashi, M.; Kawasaki, S.; Mukai, K., Experimental Check of Heisenberg ChainQuantum Statistics for a Ferromagnetic OrganicRadical Crystal. *J. Phys. Soc. Japan.* **1995**, *64* (7), 2343-2346.

93. Mukai, K.; Konishi, K.; Nedachi, K.; Takeda, K., Magnetic properties of 1, 5-dimethylverdazyl radical crystals. Ferromagnetism in 3-(4-Chlorophenyl)-1, 5-dimethyl-6-thioxoverdazyl radical crystal. *J. Phys. Chem.* **1996**, *100* (23), 9658-9663.

94. Wautelet, P.; Le Moigne, J.; Videva, V.; Turek, P., Spin exchange interaction through phenylene-ethynylene bridge in diradicals based on iminonitroxide and nitronylnitroxide radical derivatives. 1. Experimental investigation of the through-bond spin exchange coupling. *J. Org. Chem.* **2003**, *68* (21), 8025-8036.

95. Fico, R. M.; Hay, M. F.; Reese, S.; Hammond, S.; Lambert, E.; Fox, M. A., Electronic interactions in verdazyl biradicals. *J. Org. Chem.* **1999**, *64* (26), 9386-9392.

96. Gilroy, J. B.; McKinnon, S. D.; Kennepohl, P.; Zsombor, M. S.; Ferguson, M. J.; Thompson, L. K.; Hicks, R. G., Probing electronic communication in stable benzene-bridged verdazyl diradicals. *J. Org. Chem.* **2007**, *72* (21), 8062-8069.

97. Ali, M. E.; Datta, S. N., Broken-symmetry density functional theory investigation on bis-nitronyl nitroxide diradicals: influence of length and aromaticity of couplers. *J. Phys. Chem. A* **2006**, *110* (8), 2776-2784.

98. Bhattacharya, D.; Shil, S.; Misra, A.; Klein, D., Intramolecular ferromagnetic coupling in bis-oxoverdazyl and bis-thioxoverdazyl diradicals with polyacene spacers. *Theor. Chem. Acc.* **2010**, *127* (1), 57-67.

99. Dai, Y.-Z.; Dong, B.-W.; Kao, Y.; Wang, Z.-Y.; Un, H.-I.; Liu, Z.; Lin, Z.-J.; Li, L.; Xie, F.-B.; Lu, Y., Chemical Modification toward Long Spin Lifetimes in Organic Conjugated Radicals. *ChemPhysChem* **2018**, *19* (22), 2972-2977.

100. Herrmann, C.; Solomon, G. C.; Ratner, M. A., Organic radicals as spin filters. *J. Am. Chem. Soc.* **2010**, *132* (11), 3682-3684.

101. Wu, Q.-H.; Zhao, P.; Liu, D.-S., Spin Caloritronic Transport of 1, 3, 5-Triphenylverdazyl Radical. *Chin. Phys. Lett.* **2016**, *33* (3), 037303.

102. Kroto, H. W.; Heath, J. R.; O'Brien, S. C.; Curl, R. F.; Smalley, R. E., C_{60}: Buckminsterfullerene. *Nature* **1985**, *318* (6042), 162-163.

103. Akasaka, T.; Kato, T.; Kobayashi, K.; Nagase, S.; Yamamoto, K.; Funasaka, H.; Takahashi, T., Exohedral adducts of La@C_{82}. *Nature* **1995**, *374* (6523), 600-601.

104. Lu, X.; Feng, L.; Akasaka, T.; Nagase, S., Current status and future developments of endohedral metallofullerenes. *Chem. Soc. Rev.* **2012**, *41* (23), 7723-7760.

105. Kareev, I. E.; Lebedkin, S. F.; Bubnov, V. P.; Yagubskii, E. B.; Ioffe, I. N.; Khavrel, P. A.; Kuvychko, I. V.; Strauss, S. H.; Boltalina, O. V., Trifluoromethylated endohedral metallofullerenes: synthesis and characterization of Y@C_{82}(CF_3) 5. *Angew. Chem. Int. Ed.* **2005**, *44* (12), 1846-1849.

106. Zhao, J.; Huang, X.; Jin, P.; Chen, Z., Magnetic properties of atomic clusters and endohedral metallofullerenes. *Coord. Chem. Rev.* **2015**, *289*, 315-340.

107. Yi-Peng, A.; Chuan-Lu, Y.; Mei-Shan, W.; Xiao-Guang, M.; De-Hua, W., Ab initio investigations of the charge transport properties of endohedral M@C_{20} (M= Na and K) metallofullerenes. *Chin. Phys. B* **2010,** *19* (11), 113402.

108. Sato, S.; Seki, S.; Luo, G.; Suzuki, M.; Lu, J.; Nagase, S.; Akasaka, T., Tunable charge-transport properties of Ih-C80 endohedral metallofullerenes: investigation of La_2@C_{80}, Sc_3N@C_{80}, and Sc_3C_2@C_{80}. *J. Am. Chem. Soc.* **2012,** *134* (28), 11681-11686.

109. Garg, I.; Sharma, H.; Kapila, N.; Dharamvir, K.; Jindal, V., Transition metal induced magnetism in smaller fullerenes (C n for n≤ 36). *Nanoscale* **2011**, *3* (1), 217-224.

110. Rivera-Nazario, D. M.; Pinzón, J. R.; Stevenson, S.; Echegoyen, L. A., Buckyball maracas: Exploring the inside and outside properties of endohedral fullerenes. *J. Phys. Org. Chem.* **2013**, *26* (2), 194-205.

111. Wilson, L. J., Medical applications of fullerenes and metallofullerenes. *Electrochem. Soc. Interface* **1999**, *8* (4), 24.

112. Li, Y. F.; Chen, C., Fate and toxicity of metallic and metal-containing nanoparticles for biomedical applications. *Small* **2011**, *7* (21), 2965-2980.

113. Li, T.; Dorn, H. C., Biomedical applications of metal-encapsulated fullerene nanoparticles. *Small* **2017**, *13* (8), 1603152.

114. An, Y.-P.; Yang, C.-L.; Wang, M.-S.; Ma, X.-G.; Wang, D.-H., First-principles study of transport properties of endohedral Li@C_{20} metallofullerene. *Curr. Appl. Phys.* **2010**, *10* (1), 260-265.

115. Prinzbach, H.; Weiler, A.; Landenberger, P.; Wahl, F.; Wörth, J.; Scott, L. T.; Gelmont, M.; Olevano, D.; Issendorff, B. v., Gas-phase production and photoelectron spectroscopy of the smallest fullerene, C 20. *Nature* **2000**, *407* (6800), 60-63.

116. Klein, D. J.; Seitz, W. A.; Schmalz, T. G., Icosahedral symmetry carbon cage molecules. *Nature* **1986**, *323* (6090), 703-706.

117. Baei, M. T.; Soltani, A.; Torabi, P.; Hosseini, F., Formation and electronic structure of C20 fullerene transition metal clusters. *Monatsh. Chem.* **2014**, *145* (9), 1401-1405.

118. Zhao, Z.; Li, Z.; Wang, Q., Density functional theory study on the transition metal atoms encapsulated C20 cage clusters. *Mater. Res. Express* **2018**, *5* (6), 065605.

119. An, Y.-P.; Yang, C.-L.; Wang, M.-S.; Ma, X.-G.; Wang, D.-H., First-principles study of structure and quantum transport properties of C_{20} fullerene. *J. Chem. Phys.* **2009**, *131* (2), 024311.

120. Roland, C.; Larade, B.; Taylor, J.; Guo, H., Ab initio I− V characteristics of short C_{20} chains. *Phys. Rev. B* **2001**, *65* (4), 041401.

121. Wang, L.; Guo, Y.; Tian, C.; Song, X.; Ding, B., Effect of the indices of crystal plane of gold electrodes on the transport properties of C_{20} fullerene. *J. Appl. Phys.* **2010**, *107* (10), 103702.

122. Caliskan, S., Spin resolved electronic transport through $N@C_{20}$ fullerene molecule between Au electrodes: A first principles study. *Physica E Low Dimens. Syst. Nanostruct.* **2018**, *99*, 43-50.

123. Wang, B.; Wang, B.; Wei, P.; Wang, X.; Lou, W., Controlled synthesis and size-dependent thermal conductivity of Fe_3O_4 magnetic nanofluids. *Dalton Trans.* **2012**, *41* (3), 896-899.

124. Goyal, M., Shape, size and phonon scattering effect on the thermal conductivity of nanostructures. *Pramana* **2018**, *91* (6), 1-5.

125. Soyez, G.; Eastman, J. A.; Thompson, L. J.; Bai, G.-R.; Baldo, P. M.; McCormick, A. W.; DiMelfi, R. J.; Elmustafa, A. A.; Tambwe, M. F.; Stone, D. S., Grain-size-dependent thermal conductivity of nanocrystalline yttria-stabilized zirconia films grown by metal-organic chemical vapor deposition. *Appl. Phys. Lett.* **2000**, *77* (8), 1155-1157.

126. Snyder, G. J.; Toberer, E. S., Complex thermoelectric materials. *Mater. Renew. Sustain. Energy* **2011**, 101-110.

127. He, J.; Tritt, T. M., Advances in thermoelectric materials research: Looking back and moving forward. *Science* **2017**, *357* (6358).

128. Yang, J.; Aizawa, T.; Yamamoto, A.; Ohta, T., Thermoelectric properties of n-type $(Bi_2Se_3)_x(Bi_2Te_3)_{1-x}$ prepared by bulk mechanical alloying and hot pressing. *J. Alloys Compd.* **2000**, *312* (1-2), 326-330.

129. Xie, W.; Tang, X.; Yan, Y.; Zhang, Q.; Tritt, T. M., High thermoelectric performance BiSbTe alloy with unique low-dimensional structure. *J. Appl. Phys.* **2009**, *105* (11), 113713.

130. Lee, H.; Vashaee, D.; Wang, D.; Dresselhaus, M. S.; Ren, Z.; Chen, G., Effects of nanoscale porosity on thermoelectric properties of SiGe. *J. Appl. Phys.* **2010**, *107* (9), 094308.

131. Yang, N.; Chen, C.; Pan, L.; Zhao, Y.; Wang, Y., Adjustable effects of zinc substitution for indium on the thermoelectric properties of p-type CuInSe2. 02. *J. Alloys Compd.* **2020**, *847*, 156410.

132. Kihou, K.; Kunioka, H.; Nishiate, H.; Lee, C., Thermoelectric properties of yttrium-doped $Mg_3(Sb,Bi)_2$ synthesized by melting method. *J. Mater. Res. Technol.* **2021**, *10*, 438-444.

133. Butt, S.; Farooq, M. U.; Mahmood, W.; Salam, S.; Sultan, M.; Basit, M. A.; Ma, J.; Lin, Y.; Nan, C.-W., One-step rapid synthesis of Cu_2Se with enhanced thermoelectric properties. *J. Alloys Compd.* **2019**, *786*, 557-564.

134. Nieroda, P.; Leszczyński, J.; Mikuła, A.; Mars, K.; Kruszewski, M. J.; Koleżyński, A., Thermoelectric properties of Cu_2S obtained by high temperature synthesis and sintered by IHP method. *Ceram. Int.* **2020**, *46* (16), 25460-25466.

135. Bauer, G. E.; Saitoh, E.; Van Wees, B. J., Spin caloritronics. *Nat. Mater.* **2012**, *11* (5), 391-399.

136. Boona, S. R.; Myers, R. C.; Heremans, J. P., Spin caloritronics. *Energy Environ. Sci.* **2014**, *7* (3), 885-910.

137. Uchida, K.-i.; Adachi, H.; Ota, T.; Nakayama, H.; Maekawa, S.; Saitoh, E., Observation of longitudinal spin-Seebeck effect in magnetic insulators. *Appl. Phys. Lett.* **2010**, *97* (17), 172505.

138. Bader, S.; Parkin, S., Spintronics. *Annu. Rev. Condens. Matter Phys.* **2010**, *1* (1), 71-88.

139. Adachi, H.; Uchida, K.-i.; Saitoh, E.; Maekawa, S., Theory of the spin Seebeck effect. *Rep. Prog. Phys.* **2013**, *76* (3), 036501.

140. Jaworski, C.; Yang, J.; Mack, S.; Awschalom, D.; Myers, R.; Heremans, J., Spin-Seebeck effect: A phonon driven spin distribution. *Phys. Rev. Lett.* **2011**, *106* (18), 186601.

141. Jaworski, C.; Yang, J.; Mack, S.; Awschalom, D.; Heremans, J.; Myers, R., Observation of the spin-Seebeck effect in a ferromagnetic semiconductor. *Nat. Mater.* **2010**, *9* (11), 898-903.

142. Uchida, K.; Takahashi, S.; Harii, K.; Ieda, J.; Koshibae, W.; Ando, K.; Maekawa, S.; Saitoh, E., Observation of the spin Seebeck effect. *Nature* **2008**, *455* (7214), 778-781.

143. Slachter, A.; Bakker, F. L.; Adam, J.-P.; van Wees, B. J., Thermally driven spin injection from a ferromagnet into a non-magnetic metal. *Nat. Phys.* **2010**, *6* (11), 879-882.

144. Wu, S. M.; Zhang, W.; Amit, K.; Borisov, P.; Pearson, J. E.; Jiang, J. S.; Lederman, D.; Hoffmann, A.; Bhattacharya, A., Antiferromagnetic spin Seebeck effect. *Phys. Rev. Lett.* **2016**, *116* (9), 097204.

145. Sierra, J. F.; Neumann, I.; Cuppens, J.; Raes, B.; Costache, M. V.; Valenzuela, S. O., Thermoelectric spin voltage in graphene. *Nat. Nanotechnol.* **2018**, *13* (2), 107-111.

146. Li, J.; Wang, B.; Xu, F.; Wei, Y.; Wang, J., Spin-dependent Seebeck effects in graphene-based molecular junctions. *Phys. Rev. B* **2016**, *93* (19), 195426.

147. Ni, Y.; Yao, K.; Fu, H.; Gao, G.; Zhu, S.; Wang, S., Spin seebeck effect and thermal colossal magnetoresistance in graphene nanoribbon heterojunction. *Sci. Rep.* **2013**, *3* (1), 1-5.

148. Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.-e.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A., Electric field effect in atomically thin carbon films. *Science* **2004**, *306* (5696), 666-669.

149. Wu, J.; Pisula, W.; Müllen, K., Graphenes as potential material for electronics. *Chem. Rev.* **2007**, *107* (3), 718-747.

150. Pumera, M., Heteroatom modified graphenes: electronic and electrochemical applications. *J. Mater. Chem. C* **2014**, *2* (32), 6454-6461.

151. Lin, S.-Y.; Lin, Y.-T.; Tran, N. T. T.; Su, W.-P.; Lin, M.-F., Feature-rich electronic properties of aluminum-adsorbed graphenes. *Carbon* **2017**, *120*, 209-218.

152. Goswami, T.; Panda, A.; Klein, D. J., Spin-Density Localization in Graphene at Boundaries and at Vacancy Defects. *J. Phys. Chem. C* **2019**, *123* (14), 9479-9485.

153. Xu, Y.; Li, Z.; Duan, W., Thermal and thermoelectric properties of graphene. *Small* **2014**, *10* (11), 2182-2199.

154. Saroka, V.; Batrakov, K.; Demin, V.; Chernozatonskii, L., Band gaps in jagged and straight graphene nanoribbons tunable by an external electric field. *J. Condens. Matter Phys.* **2015**, *27* (14), 145305.

155. Zheng, H.; Liu, H.; Tan, X.; Lv, H.; Pan, L.; Shi, J.; Tang, X., Enhanced thermoelectric performance of graphene nanoribbons. *Appl. Phys. Lett.* **2012**, *100* (9), 093104.

156. Ouyang, Y.; Guo, J., A theoretical study on thermoelectric properties of graphene nanoribbons. *Appl. Phys. Lett.* **2009**, *94* (26), 263107.

157. Sevinçli, H.; Cuniberti, G., Enhanced thermoelectric figure of merit in edge-disordered zigzag graphene nanoribbons. *Phys. Rev. B* **2010**, *81* (11), 113401.

158. Mazzamuto, F.; Nguyen, V. H.; Apertet, Y.; Caër, C.; Chassat, C.; Saint-Martin, J.; Dollfus, P., Enhanced thermoelectric properties in graphene nanoribbons by resonant tunneling of electrons. *Phys. Rev. B* **2011**, *83* (23), 235426.

159. Lee, H.; Son, Y.-W.; Park, N.; Han, S.; Yu, J., Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states. *Phys. Rev. B* **2005**, *72* (17), 174431.

160. Pisani, L.; Chan, J.; Montanari, B.; Harrison, N., Electronic structure and magnetic properties of graphitic ribbons. *Phys. Rev. B* **2007**, *75* (6), 064418.

161. Huang, B.; Liu, M.; Su, N.; Wu, J.; Duan, W.; Gu, B.-l.; Liu, F., Quantum manifestations of graphene edge stress and edge instability: A first-principles study. *Phys. Rev. Lett.* **2009**, *102* (16), 166404.

162. Li, G.; Yoon, K.-Y.; Zhong, X.; Wang, J.; Zhang, R.; Guest, J. R.; Wen, J.; Zhu, X.-Y.; Dong, G., A modular synthetic approach for band-gap engineering of armchair graphene nanoribbons. *Nat. Commun.* **2018**, *9* (1), 1-9.

163. Yang, W.; Lucotti, A.; Tommasini, M.; Chalifoux, W. A., Bottom-up synthesis of soluble and narrow graphene nanoribbons using alkyne benzannulations. *J. Am. Chem. Soc.* **2016**, *138* (29), 9137-9144.

164. Li, G.; Yoon, K. Y.; Zhong, X.; Zhu, X.; Dong, G., Efficient Bottom-Up Preparation of Graphene Nanoribbons by Mild Suzuki–Miyaura Polymerization of Simple Triaryl Monomers. *Chem. Eur. J.* **2016**, *22* (27), 9116-9120.

165. Wierzbicki, M.; Swirkowicz, R.; Barnaś, J., Giant spin thermoelectric efficiency in ferromagnetic graphene nanoribbons with antidots. *Phys. Rev. B* **2013**, *88* (23), 235434.

166. Zeng, M.; Feng, Y.; Liang, G., Graphene-based spin caloritronics. *Nano Lett.* **2011**, *11* (3), 1369-1373.
167. Chico, L.; Orellana, P.; Rosales, L.; Pacheco, M., Spin and charge caloritronics in bilayer graphene flakes with magnetic contacts. *Phys. Rev. Appl.* **2017**, *8* (5), 054029.
168. Shirdel-Havar, M.; Farghadan, R., Spin caloritronics in spin semiconducting armchair graphene nanoribbons. *Phys. Rev. B* **2018**, *97* (23), 235421.