Appendix A

In this chapter, we briefly discuss the structural behavior of DNA and the dynamics of denaturation of DNA.

The structure of DNA

DNA polymer is assembled by molecules called nucleotides which are the building blocks of nucleic acids. Each nucleotide has a phosphate group, a sugar group and a nitrogenous base, as shown in Figure 5.17. There are four types of nitrogenous bases, Adenine (A), Thymine (T), Guanine (G) and Cytosine (C). The genetic

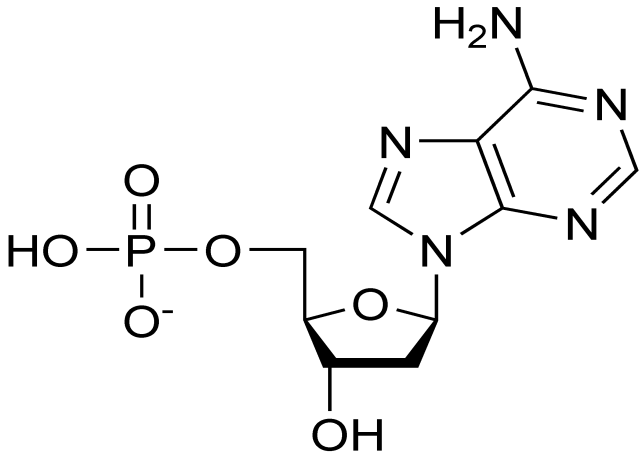


Figure 5.17: Nuleotide: The monomer of DNA polymer strand. The phosphate and carbonic base are bonded by covalent bond with the sugar. Image taken from *Wikipedia*.

codes of DNA build upon on the sequence order of these four bases. Genes can be made from few hundred DNA bases to more than 2 million bases according to the task that it has to perform. Putting the right alphabet one by one, we can create a word which holds a meaning and on the same way putting these word

in a proper way we can build a sentence which is called language, quite similarly the order of nitrogen bases (A,T,G,C) of a DNA chain create a language for the cell [8, 158, 222, 223]. It is noticed that the sequence of genes mostly same in all people and a few percent, about less than 1 percent of the entire genes are slightly different still these minor changes in sequence of genes makes a person unique [8, 22, 224, 225]. The nitrogen bases can be classified into two categories, two-ringed purines and single-ringed pyrimidines. Adenine(A) and Guanine (G) nitrogen bases belong to the purine category as they hold a double-ring structure with a six-carbon ring fused to a five-carbon ring. Cytocine (C) and Thymine(T) belongs to Pyrimidine class as they have only a six-carbon ring structure[1]. The chemical structure of these bases is shown in Figure 5.18. These nucleotides make a

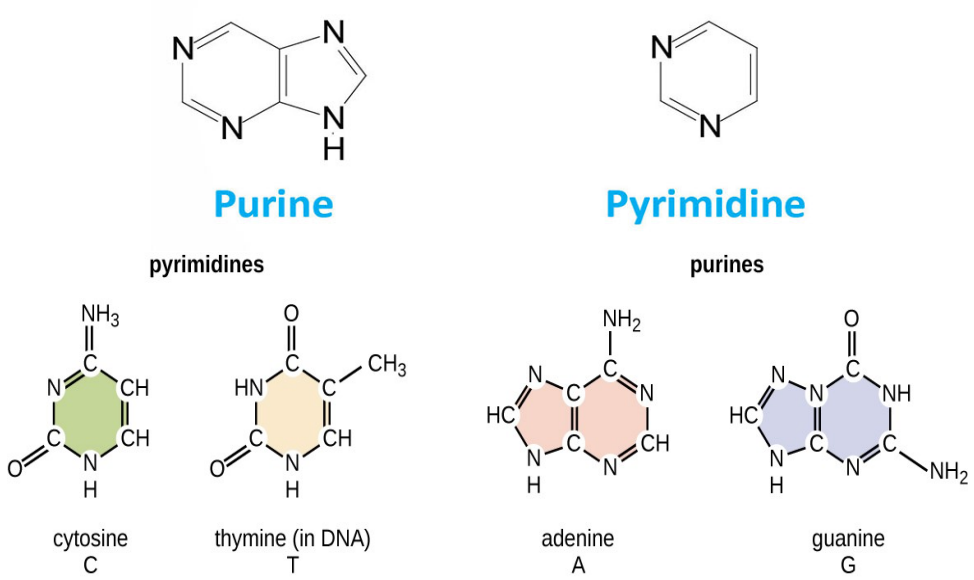


Figure 5.18: Nitrogenous bases: The two-ringed purines (Adenine and Guanine) and the single-ringed pyrimidines (Cytosine and Thymine). Thymine is unique to DNA. The diagram credit goes to 'The Medical Biochemistry Page','Lumen Learning'.

chain with the interaction of covalent bonds between the deoxyribose sugar of one nucleotide and the phosphate group of the following bases. This arrangement forms a polymer chain with the sugar-phosphate backbone. DNA makes itself antiparallel that means the two strands directionally point opposite to each other due to reverse orientation of the sugar molecule. The phosphate groups make a bond with the 3^{rd} or $5th$ carbon atoms of adjacent sugar rings [8, 158, 224, 226–228], and that

[1]Uracil (U) belongs to RNA molecule, instead of thymine (T) in DNA. It is also Pyrimidine by nature

gives DNA a direction as shown in Figure 5.19. The two strands of DNA twist

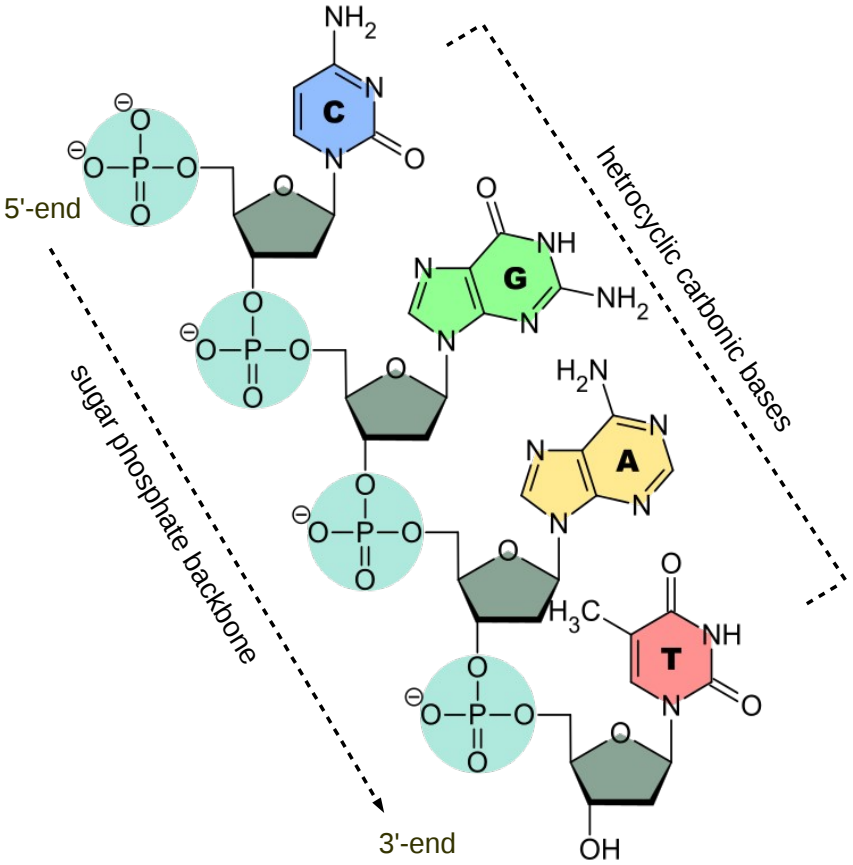
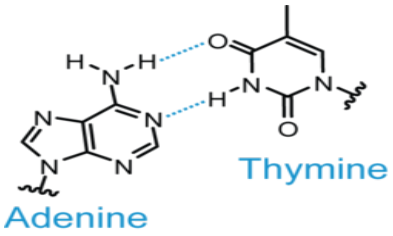


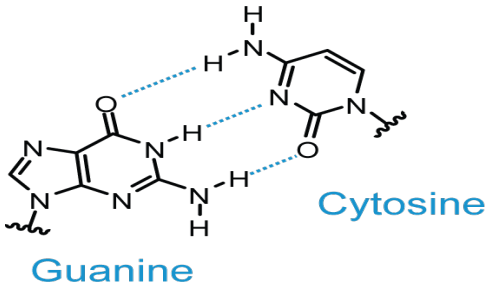
Figure 5.19: The basic structure of DNA, (single *strand*). There is a typical way of numbering carbons of an organics compound for referring and that gives a direction here 5-prime and 3-prime. Here the DNA strand shows 5' $->$ 3' direction. *Image taken from Wikipedia Commons.*

around each other and make a right-handed helix. That handedness creat grooves and their orientation. The twisting geometry of the DNA builds a wider gap that is called major groove and a narrower gap that is called minor groove, as shown in Figure 5.20(b). The phosphate group repeats each time with one nitrogen base among A,T,G,C [8, 158, 222, 226, 229]. A purine on one strand makes a bond with a pyrimidine of the other strand through hydrogen bonds[9, 22, 52, 222, 230].

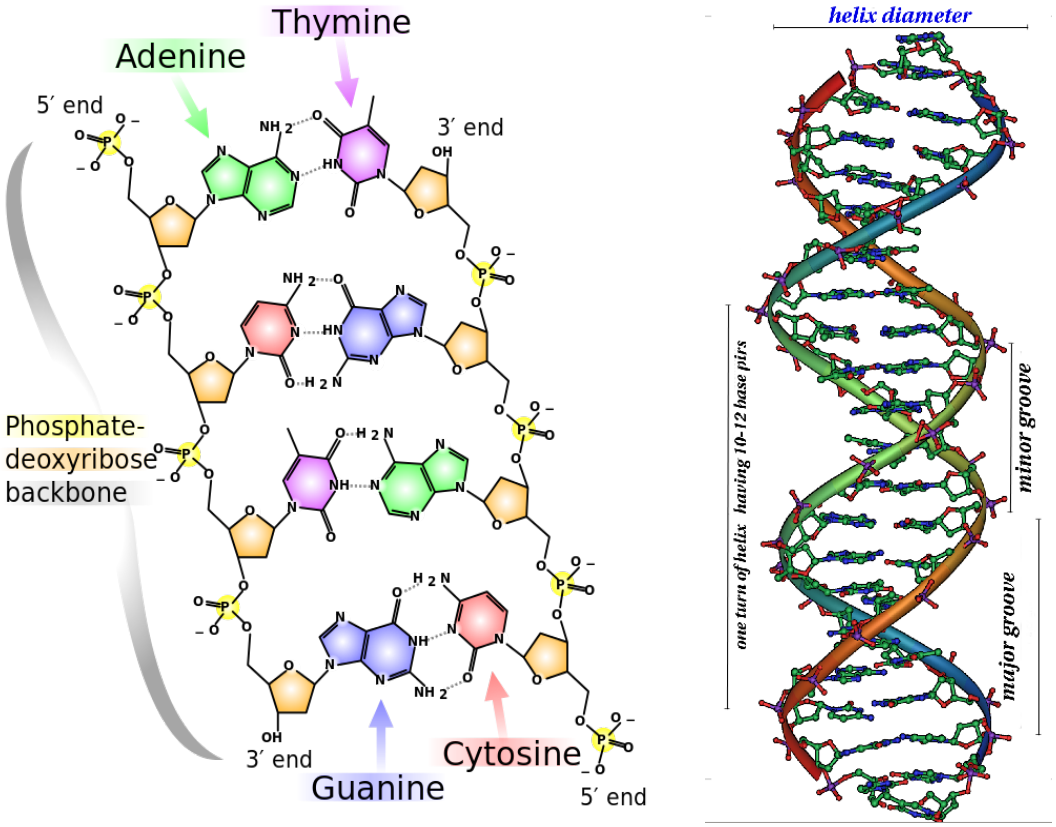
1. Adenine(A) bonds with Thymine(T) (through 2 hydrogen bonds).



2. Guanine(G) bonds with Cytocine(C) (through 3 hydrogen bonds).



In a DNA molecule there is an equal number of purine and pyrimidine residues. The four nitrogen bases A, T, G, and C are not found in equal number but the number of A should be always equal to the number of T, and the number of G should be always equal to the number of C according to the Chargaff's rules [231, 232] for the Watson and Crick's model of the DNA double helix. Figure 5.20(a) shows a complete DNA chain with all the properties that have discussed above. A question that always asked related to DNA structure and that is 'why double helix'? Thermodynamic stability is the critical reason for this double helix structure of DNA. Since solubility is a chemical property hence the solubility of different parts of DNA are different in the water. The sugar and phosphates are hydrophilic(water-soluble) in nature, and the nitrogen bases (A,T,G,C) are hydrophobic in nature(not water-soluble). Most of the space in the cells are filled by water, so the bases place themselves in the center, and the sugar-phosphate backbone of DNA stay outside. Now to suppress the space entirely, it has to twist considering all the neighbor atoms movement around a common central axis, each base pair gets a rotation of around 35° concerning the previous one, and then the DNA strand turns out into the famous double helix structure [8, 158, 224, 226]. There are several possible conformations of DNA that are observed in various forms based on the environmental conditions. The differentiations are mainly in spacing between nucleotides and number of nucleotides per turn, rotation per



(a) Complementary strands of a DNA (b) DNA double helix structure

Figure 5.20: The structure of DNA. (a) Covalent bonds between the phosphate of one nucleotide and the sugar of the next nucleotide are shown by solid lines, and hydrogen bonds between bases are shown by dashed lines. (b) Double helical structure of DNA in B-form. *Image taken from Wikipedia Commons.*

base pair, vertical rise per base pair and in helical diameter. The most common form of duplex DNA that is proposed by Watson and Crick and it is B-form. Naturally DNA double helices are classified into A, B and Z-types. B-DNA is a right handed helix and it holds about 10 nucleotide per turn. A-form of DNA holds 11 phosphates and Z-form holds 12 phosphates per turn. These slight differences are also significant in biology. A-DNA is right handed helix but the Z-DNA shows left handedness so it is assigned -12 phosphates per turn for Z-DNA rather than +12 phosphates like A and B-DNA. The differentiations are shown in Table 5.4.

All these forms of DNA maintain Chargaffs rule so the number of A always be equal to the number of T, and the number of G always be equal to the number of C [231, 232].

Geometry attribute	A-form	B-form	Z-form
Orientation	Right-handed	Right-handed	Left-handed
Helix diameter	2.3 nm	2.0 nm	1.8 nm
Helix twist(Rotation/bp)	32.7^0	34.3^0	-30.0^0
bp/turn	11	10	-12
Inclination of bp to axis	$+19^0$	-1.2^0	-9^0
Topology of major groove	Wide,deep	Narrow,deep	Flat
Topology of minor groove	Narrow,shallow	Broad,shallow	Narrow,deep

Table 5.4: Comparison geometries of the most common DNA forms.

DNA dynamics

The cell cycle is the life cycle of a living being. A mother cell splits into two or more daughter cells in an organised series of steps that is called cell cycle. It is called a cycle because after a certain time the two daughter cells will be involved in the exact same process of division. As the genetic information is stored in the DNA so at the time of cell division making copies of the DNA is the key part. This process is done mainly in two ways: Transcription and Replication. In this section these two process are briefly discussed here.

DNA replication

The first step towards cell division starts with each double strands DNA breaks into two single strands. This single strand now beacomes a template for making a new strand and a complementary strand making process according to that template sequence is called DNA replication. As a result each daughter cell gets its own complete genome. The replication process, shown schematically in Figure 5.21. The process is directed by an enzyme called DNA polymerase enzyme. The replication process starts with unzipping of double strand into two single strands. The hydrogen bonding between the base pairs of DNA is broken by an enzyme known as DNA helicase and the DNA chain unzips like the Y shape form that is known as replication fork. The replication fork functions in two directions(bi-directional) as the direction of synthesis of one strand is the same direction to the growing of the replication fork(3' to 5' direction) and the other strand is synthesized in the opposite to the direction of the growing replication fork(5' to 3' direction). The strand which is oriented in the 3' to 5' direction is called leading strand and the

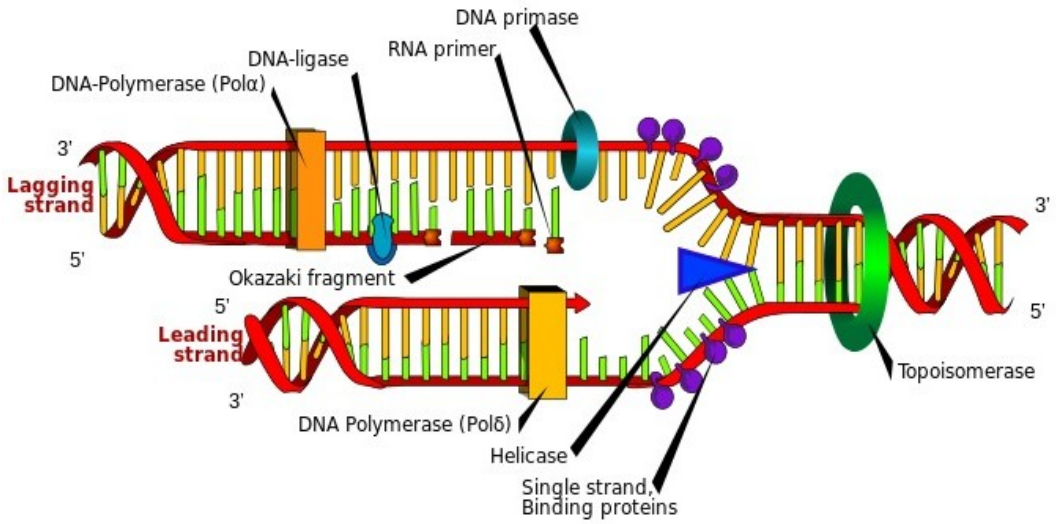


Figure 5.21: Schematic representation of DNA replication process, Double strands split into two single strand and each single strand acts as a template for making the complementary strand for each of them. *Image taken from Wikipedia Commons*

other one which is oriented in the 5' to 3' direction is called lagging starnd. The lagging strand is synthesized in short segments called Okazaki fragments. These short sequences are linked together by an enzyme called DNA ligase and creat the lagging strand. An enzyme called DNA primase, reads the lagging strand template and initiates synthesis of a short complementary RNA primer [8, 22, 224, 226]. A DNA polymerase extends the primed segments and forms the Okazaki fragments. The replication fork is shown schematically in Figure 5.22.

DNA transcription

Transcription is a process in which the template of a particular segment of DNA is duplicated into a messenger RNA by an enzyme called RNA polymerase.The complementary RNA strand is called a primary transcript [8, 22, 224, 226]. The complementary RNA strand replaces thymine(T) to the uracil(U). The stability of base pairs supposes to only a limited extent so that the helix can be unzipped at the proper time through enzyme. After transcription RNA polymerase has the ability to close the base pair also. The processes are done in a synchronized way [226, 233]. The process is shown in Figure 5.23. In the above discussion of replication and transcription process it is found that double helix structure has several advantages. One of the most relevant aspect of this structure is that it is suitable for the replication and transcription process.

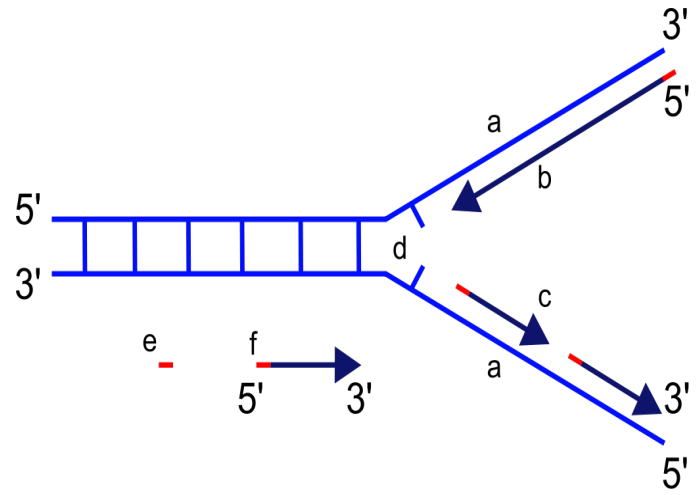


Figure 5.22: Schematic representation of replication fork. a: template, b: leading strand, c: lagging strand, d: replication fork, e: primer, f: Okazaki fragments. *Image taken from Wikipedia Commons*

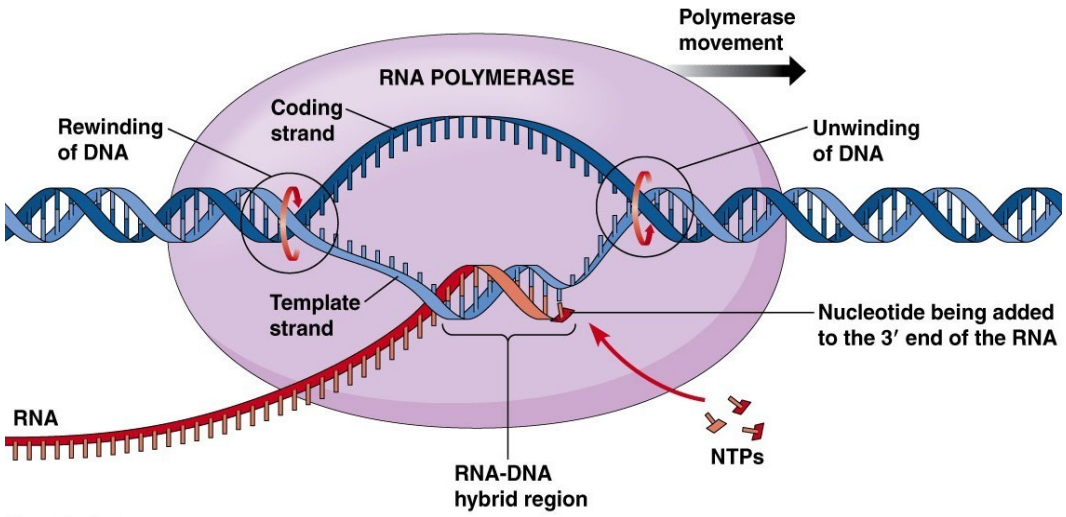


Figure 5.23: The figure shows the process of DNA transcription. Sequence is copied by mRNA as template. *Image taken from Wikipedia Commons*

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List of Publications and Presentations

International Journals:

- *"Melting of DNA in confined geometry"*
  Arghya Maity and Navin Singh ,
  European Biophysics Journal ,(Accepted), (2020)

- *"Stability of DNA passing through different geometrical pores"*
  Arghya Maity, Amar singh and Navin Singh,
  Europhysics Letters (EPL), **127** 28001 (2019)

- *"Differential stability of DNA based on salt concentration"*
  Arghya Maity, Amar Singh and Navin Singh,
  European Biophysics Journal, **46** 33−40 (2017)

- *"How Geometry of the Confinement impacts on DNA Movement in Molecular Dynamics Simulations"*
  Arghya Maity, Petra Imhof and Navin Singh,
  (manuscript under preparation)

Conference proceedings in International Journals:

- *"DNA denaturation in ionic solution"*
  Arghya Maity, Amar Singh and Navin Singh,
  AIP Conf. Proc. **1728** 020415 (2016)

List of conferences/schools attended/participated:

- *"PURI POLYMER CONFERENCE 2018"*,
  December 12 -14, 2018, Institute of Physics, Bhubaneswar, INDIA.
  Oral Presentation

- *"INTERNATIONAL CONFERENCE ON CONDENSED MATTER & APPLIED PHYSICS (2015)"*
  October 30-31, 2015, Bikaner, Rajasthan, INDIA.
  Poster Presentation

- *"Conference on DNA Physics 2017"*,
  March 09-11, 2017, BITS-Pilani, Rajasthan, INDIA.

- A workshop on *"Statistical Physics of Soft Matter"*,
  $25^{th} - 30^{th}$ November, 2015, BHU, Varanasi, INDIA.

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Mr. Arghya Maity pursued his B.Sc degree in Physics honours from Vidyasagar University, West bengal then Master's degree at School of Physics at Sambalpur University, Odisha, India. He worked in UGC-DAE Consortium for Scientific Research, Kolkata for his M.Sc research project. He joined Department of Physics, BITS Pilani as a Research Scholar in January 2015. He is pursuing a Ph.D. degree now. He has published several research papers, including letters, and few are under review. His research interests are in the areas of Biopolymers, Statistical Mechanics and Quantum Biology. He has achieved many international scholarships like,"*Mexican Council of Science (CONACyT) Ph.D. Scholarship*" & "*Free University of Berlin Ph.D. sandwich fellowship*". He has worked in Germany at Department of Physics, Free University of Berlin lab with Prof. Petra Imhof. In addition to this, he has participated and presented his work in several national and international conferences of high repute.