

Preface

The thesis presents a theoretical study on the stability of the DNA molecule in different confined environments and concentrated solutions. DNA always experiences a different type of geometrical confinement because of the cell environment. So it is essential to study the behaviour of the DNA in these confined geometries. For the studies, we consider a statistical model called the Peyrard Bishop Dauxois model popularly known as the PBD model. Additionally, we simulate DNA in different confined geometry through the molecular dynamics simulation method to study the dynamics also. Salt is also a significant contributor to cell activities. The primary role of salt in the cell is to provide stability to the DNA molecule by shielding the repulsion between two negative strands of DNA. However, beyond a particular value of salt concentration, the DNA molecule displays a contrary behaviour *in vivo* as well as *in vitro*. Recent experimental studies deeply motivate the present thesis work. Our findings are in close agreement with the experimental results.

The stability of DNA molecules during the encapsulation process is a topic of intense research. We have studied the stability of DNA in different confined geometries. Our results show that not only the confinement but also the geometry of the confined space plays a prominent role in the stability and opening of the molecule. The recent years witnessed significant advances in nanopore technology and DNA sequencing. Our studies also try to explain these issues.

To the reader

I write the thesis in “we” form. Sometimes this may appear strange to the reader, as the thesis is of a single author. Since the published work is written in “we” form, I find it convenient to write the complete thesis in “we” form.

Thesis outline

The thesis is divided into five chapters and one additive work named Future Scope: Following Research Work. The first two, respectively, are meant as background to the particular fields in biology and physics studied. In chapters 3-5, we discuss the research work that has been

carried out. Here is a brief discussion about the organization of the thesis.

- In **chapter 1**, we discuss the DNA synthesis in-vitro. Then we present a detail literature review of the theoretical, as well as the experimental studies that are related to our work.
- In **chapter 2**, we discuss the methodology we have used to study the research problems we have taken.
- In **chapter 3**, we study the differential stability of DNA in the concentrated solutions.
- In **chapter 4**, we explore the DNA stability in different confined geometry on the thermal ensemble.
- **Chapter 5**, we discuss the stability of DNA, which is passing through different geometrical pores.
- The research work is summarized in **Conclusions and Following Research Work**.
- We also study the time evolution of the DNA molecule confined in cylindrical geometry. Using GROMACS, we evaluate the conformational properties of the DNA molecule. The work is under progress, and hence, we decided to report as a **Future Scope: Following Research Work**.
- The structure of DNA and DNA dynamics is discussed in **Appendix A**.