
Departmental Seminar

An overview of structural studies performed on some biologically important macromolecules

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The 3D-structures of biologically important macromolecules (DNA, RNA, proteins, and graphene) are significant in understanding their biological roles. Over the past decade unusual nucleic acids such as four stranded DNA helices consisting mainly of H:W base pairing, RNA bulge motifs containing unpaired bases and pseudo-continuous helices have gained huge importance for their functional role in various biological processes^{1,2}. Along with nucleic acids, proteins are also present inside the nucleus of a cell. The A and B-type lamins are the major intermediate filament proteins conferring proper shape and mechanical rigidity to the nucleus³. We have performed structural studies on such unusual nucleic acids and A-type lamin proteins by MD and SMD simulations. Furthermore, widespread disease conditions have prompted researchers to indulge more into drug discovery and thereby developing appropriate drug-carrying vehicles. An important drug-carrying vehicle is graphene, as it has both hydrophobic and hydrophilic properties along with some unique physicochemical properties. Thus, we have tried to study some features of this material focusing particularly on tearing of GO sheets by quantum chemical calculations.

References:

1. Hermann, T.; Patel, D. J. *Struct Fold Des* 2000, 8, R47-R54.
2. Bochman, M. L.; Paeschke, K.; Zakian, V. A. *Nat Rev Genet* 2012, 13, 770-780.
3. Dechat, T.; Adam, S. A.; Taimen, P.; Shimi, T.; Goldman, R. D. *Cold Spring Harb Perspect Biol* 2010, 2, a000547.

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2:00 PM (Tea/Coffee at 1:45 PM)

Seminar Hall, TCIS