

Seminario de Química Física



Jueves 11 de julio de 2024 – 12:00 h



Salón de Actos de la Biblioteca

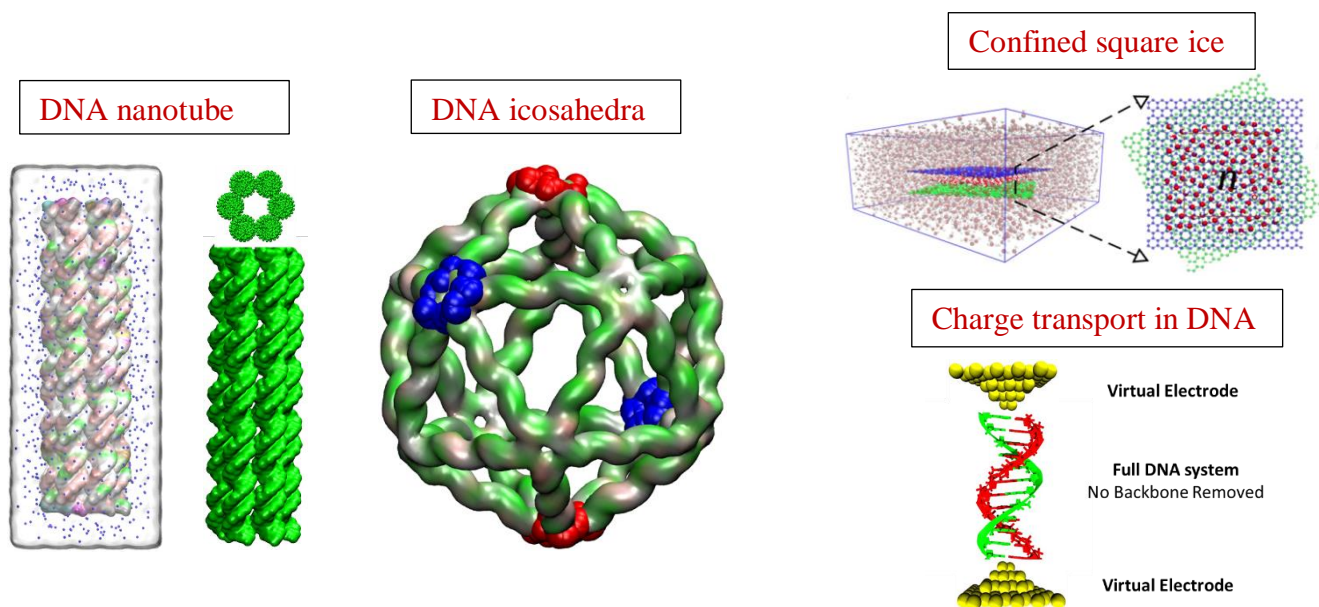
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Multiscale modelling of complex systems

Computer simulations are important scientific tools to understand the emergence of collective properties from chemical structures in complex molecular systems. It has helped us in improving our basic understanding and providing calculation tools for the pre-synthesis design and screening of novel materials for various technologies. In this talk I will summarize our efforts in understanding the structure and dynamics confined fluid, self-assembly and mechanics of various DNA molecules and charge transport in molecular system.



1. J Majumdar, S Dasgupta, S Mandal, M Moid, M Jain, Prabal K Maiti, *The Journal of Chemical Physics* 158 (3), 034501 (2023).
2. Hemant Kumar, Saheb Bera, Subhadeep Dasgupta, AK Sood, Chandan Dasgupta, and Prabal K Maiti, *Physical Review B* 107 (16), 165402 (2023).
3. Abhishek Aggarwal, Saientan Bag, Ravindra Venkatramani, Manish Jain, Prabal K. Maiti, *Nanoscale*, 12, 18750 (2020).
4. Himanshu Joshi, Atul Kaushik, Nadrian Seeman and Prabal K Maiti, *ACS Nano*, 10, 7780 (2016).