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Low-energy electrons and DNA: A perspective from first-principles simulations

Thursday 8 September 2022 11:00 (40 minutes)

In this talk I will provide a general overview on the role played by low energy electrons in DNA damage.First, I willbriefly discussexperimental findings and theoretical results hand in hand with the aim of describing the-physics and chemistry that occurs during the process of radiation damage, from the initialstages of electronic excitation, through the inelastic propagation of electrons in the medium,the interaction of electrons with DNA, and the chemical end-point effects on DNA in a realistic, physiological environment.The role played by the aqueous solution and the amino acids from the histones in chromatinwill be considered as well as thermal fluctuations. The focus of this talkwill be our recent first-principlesmolecular dynamics simulations that address the issue of how the environment favoursor prevents LEEs from causing damage to DNA [1,2]. I will finish by summarising the conclusionsachieved so far, and by suggesting several possible directions for further study.

REFERENCES
[1] J. Kohanoff, M. McAllister, G. Tribello, and Bin Gu, Interactions between low energy electrons and DNA: A perspective from first-principles simulations, J. Phys.: Condens. Matter 29, 383001 (2017).
[2] M. McAllister, N. Kazemigazestane, L. T. Henry, Bin Gu, I. Fabrikant, G. A. Tribello, and J. Kohanoff, Solvation Effects on Dissociative Electron Attachment to Thymine, J. Phys. Chem. B 123, 1537 (2019).

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