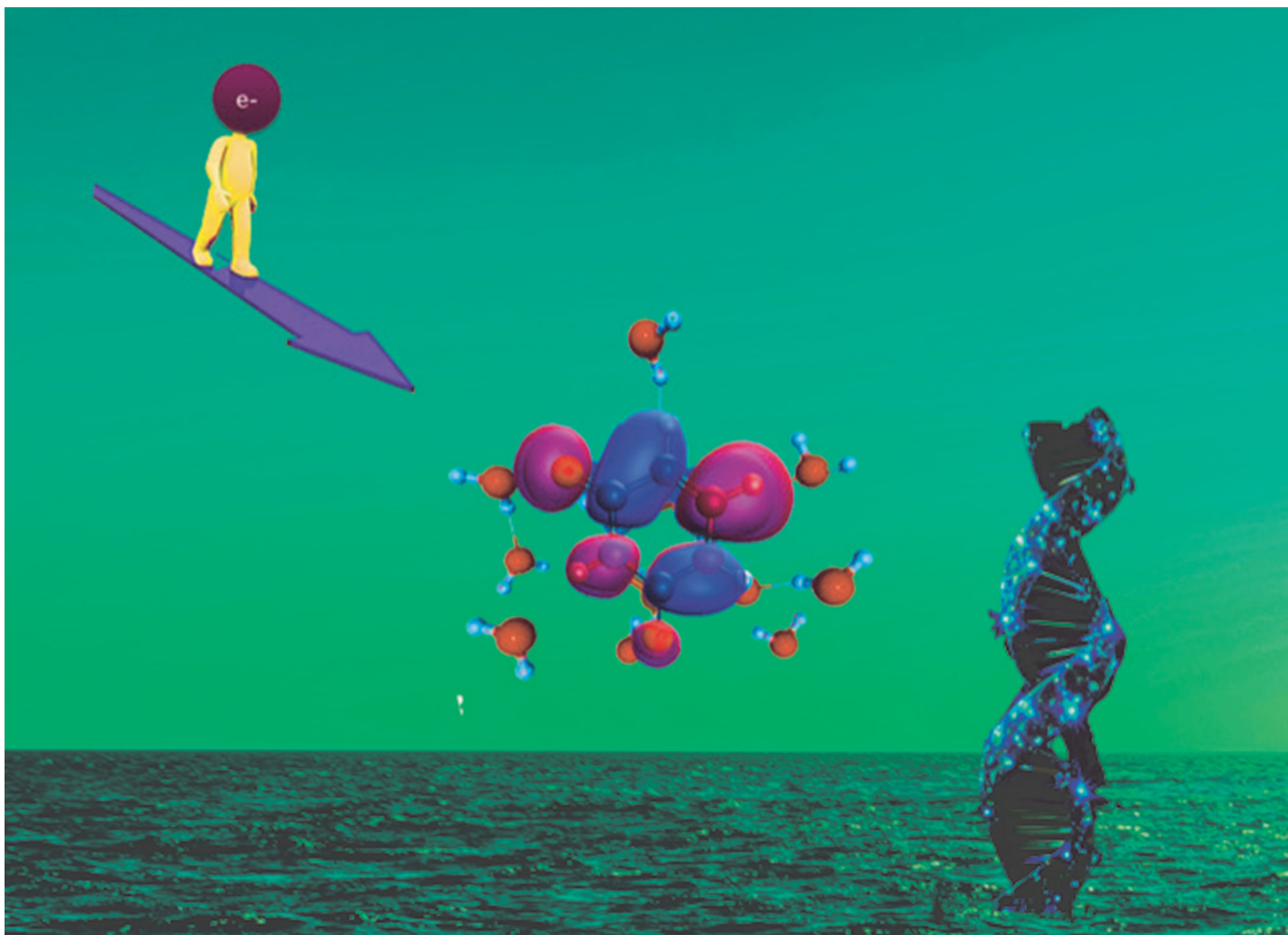


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Showing research from Dr Spiridoula Matsika's group,
Department of Chemistry, Temple University, Philadelphia,
PA, USA.

Impact of solvation on the electronic resonances in uracil

This study examines computationally the effect of aqueous solvation on electronic resonances formed by electron attachment to uracil. The work is part of an effort to understand how electrons created by radiation interact with the building blocks of nucleic acids and eventually lead to strand breaks. Using solvated uracil configurations obtained from molecular dynamics and electronic structure methods it was found that resonances generated by attaching an electron to π^* orbitals in uracil are greatly affected by solvation structure.

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