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Transient Anion States of Biomolecules¹

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Much of the interest on electron interactions with biomolecules is related to radiation damage [Gohlke and Illenberger, *Europhys. News* **33**, 207 (2002)]. The high energy photons employed in radiology and radiotherapy generate a large number of fast electrons in living cells. These electrons thermalize in a picosecond scale, eventually forming dissociative metastable anions with water and biomolecules. In this work, we employ the parallel version of Schwinger Multichannel Method with Pseudopotentials [Bettega *et al.*, *Phys. Rev. A* **47**, 1111 (1993); Santos *et al.*, *J. Phys. Chem.* **136**, 084307 (2012)] to investigate transient anion states of protein and nucleic acid precursors. We address glycine in both neutral and zwitterionic forms, as well as glycine-water clusters and disulfide bonds. The interest on the two forms of glycine (and other amino acids) relies on the fact that only the neutral form is stable in the gas phase, while the zwitterion is more stable in solution, pointing out limitations of standard gas-phase studies. Electron attachment to disulfide bonds also has potential impact on protein stability. Finally we address transient anion states of substituted uracil molecules in the gas phase.

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