Theoretical study of positron binding and annihilation properties of biomolecules in solution

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Positronic compounds have been extensively discussed in the last decade in theoretical and experimental studies [1]. In recent years, the interest in positron attachment to small biomolecules solvated was motivated by the applications of positrons in medicine as the Positron Emission Tomography (PET) [2] and the positron annihilation with core electrons in biological environment to positron-based cancer therapy [3]. The existing theoretical studies about solvated positronic molecules are limited to small clusters, and the bulk effects on positron attachment still need to be better understood [4]. This work investigates the positron binding ability and annihilation rates, including the solvent effect for the amino acids glycine, alanine, and proline. Our results considering large clusters indicate an intense competition between the solute and solvent for the positron, raising a question on the existence of solvated positronic molecules.

References

- 1. G. F. Gribakin et al., Rev. Mod. Phys. 82, 2557 (2010).
- 2. P. Moskal et al., Physics in Medicine & Biology 64, 055017 (2019).
- 3. K. Shibuya et al., Communications Physics 3, 1 (2020).
- 4. K. Suzuki et al., J. Phys. Chem. A **123**, 1217 (2019).