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Photoemission and state-selected fragmentation of "aromatic cyclo-dipeptides"in the gas-phase

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Linear (ℓ-) and cyclo (c-) dipeptides built by linking two aminoacids via one/two peptide bonds, are the simplest peptides present in nature. They are the object of widespread interest since the 50s of the previous century due to their central role in several areas such as development of therapeutics[1] and preparation of nanostructured materials[2]. It has also been proposed that c-dipeptides may have played a role in the emergence of life in the early universe[3] thanks to both their capability to withstand radiation and to produce crucial intermediates for the development of peptide chains[4]. Moreover, among the ℓ- and c-dipeptides the ones containing an aromatic aminoacid in the side chain are of interest for the study of the dynamics involving energy and charge transfers[5] in bio-systems.
In this work we present a combined experimental and theoretical study of the electronic structure and state-selected fragmentation of three different c-dipeptides containing aromatic aminoacids in the side chains.
A systematic *ab-initio* study implemented with different computational methods allowed to explore geometry, energy levels, electronic wave-functions and optical properties of c-GlyPhe, c-TrpTrp and c-TrpTyr. Valence photoemission (PES), mass spectrometry (MS) and photoelectron-photoion coincidence, PEPICO, measurements have been performed at the CIPO beamline[6] of Elettra synchrotron facility. From the comparison between the calculated density of states (DOS) and the experimental PES spectra typical fingerprints due to the presence of the aromatic side chain have been identified in all the three samples[7], evidencing the key role of the side chain in determining the photo-chemical properties of this class of molecules. The correlation between the electronic distribution of the molecular orbitals and the production of certain fragments has been investigated via PEPICO experiments, allowing us to obtain information on fragmentation pathway versus binding energy (BE) as well as approximate onsets for the production of specific fragments and correlation among different channels.

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