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From core to valence states: a comprehensive experimental and theoretical photoelectron spectroscopy study of proteinogenic amino acids

Amino acids (AAs) are fundamental building blocks of life. In the solid state, AAs are of considerable scientific and technological interest due to their widespread use in the food and pharmaceutical industries. Despite this, most spectroscopy studies focus on gas-phase species or surface adsorbates, while crystalline AAs remain underexplored, largely because of experimental challenges associated with radiation damage.

A detailed understanding of chemical bonding in solid-state AAs, encompassing both intra- and inter-molecular interactions, is nevertheless of great interest. Photoelectron spectroscopy provides access to this information, however, spectra are often complex and difficult to interpret. This motivates a combined experimental-theoretical approach, in which density functional theory (DFT) is used to calculate simulated spectra based on known crystal structures. Composed primarily of light elements, readily available in high purity and crystallinity, and exhibiting systematic variation in key chemical motifs, proteinogenic AAs constitute an ideal model system for validating the robustness of such an integrated experiment-theory framework.

Photoelectron spectroscopy measurements, including core, semi-core, and valence states, form the experimental basis with a particular focus on the mitigation of radiation damage. Calculated relative core binding energies show excellent agreement with experiment and enable reliable assignments. Projections of the density of states provide insight into the influence of local coordination and extended crystal structure, yielding a systematic understanding of the electronic structure and bonding in solid-state AAs.

This work presents a computationally efficient strategy for unlocking the information encoded in experimental photoelectron spectra and lays the foundation for a broader application of theory-assisted photoelectron spectroscopy.

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