Electronic Structure of the Nucleobases

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Abstract

We present a comparison between experimental and calculated soft X-ray spectr of DNA's nucleobases, adenine (A), guanine (G), cytosine (C), and thymine (T) using X-ray absorption spectroscopy (XAS) and soft X-ray emission spectroscop (XES). Spectra of the 1s thresholds of carbon, nitrogen, and oxygen give a complete picture of the occupied and unoccupied partial density of states of the nucleobases. A combination of both Hartree–Fock and density functional theory calculations are used in the comparison to experimental results. Most experimental results agree well with our theoretical calculations for the XAS and XES of all bases. All spectral features are assigned. A comparison of the

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