The Number of High-Energy Bands in the Photoelectron Spectrum of Alkanes

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It was observed that within the Bieri-Dill-Heilbronner-Schmelzer model for the calculation of the ionization energies of alkanes C_nH_{2n+2}, there are exactly n C_{2s}-electron energy levels lying below the degenerate $\alpha - \beta$ manifold. We now show that, indeed, this regularity is obeyed by practically all alkane species. Exceptions do exist, but they must possess a (chemically infeasible) group of more than six mutually connected quaternary carbon atoms.

Key words: Hydrogen filled Molecular Graph; Inertia; Laplacian Spectrum.