Unusual definition of electronic structure of molecules and organic semiconductors on optical properties

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The definition of such characteristics as first ionization potential (**IP**) and electron affinity (**EA**) of molecules and organic semiconductors is a significant problem of nanoelectronics and nanomaterials. In our previous works [1-3] methods for determination electronic structure of molecules and materials using **Electron phenomenological spectroscopy** (**EPS**) were shown. Unlike conventional spectroscopic methods, the **EPS** studies substances as a comprehensive quantum continuum without separating the spectrum of the substance into characteristic spectral bands on certain frequencies or wavelengths of individual functional groups or components. **EPS** [1] is based on the correlations between integral optical characteristics and properties of substance as a single whole quantum continuum: *spectrum-properties* and *color-properties*. Qualitatively, new laws appear on the integral level. New physicals phenomena appear in consideration of the integral systems which absorb radiation. These allow the use of **EPS** methods for studying individual and complex multicomponent substances.

Unlike our previous works [2-3] within **EPS** we present new methods for determination of the electronic structure. The developed methods have been proved by a big amount of objects – aromatic and heteroatomic compounds. The first of them [4] is a remote method based on color characteristics definition of the photoimages of the investigating objects. The second method [5] is based on the combination of optical and topological properties of organic molecules:

$$IP = A_0 + A_1 \cdot q_{photo},\ EA = B_0 + B_1 \cdot q_{photo},\ IP = C_0 + C_1 \cdot \Theta + C_2 \cdot I,\ EA = D_0 + D_1 \cdot \Theta + D_2 \cdot I$$

here q_{photo} –color characteristic of the photoimage in RGB colorimetric system; A_0, A_1, B_0, B_1 – empirically determined coefficients, depending only on the type of color characteristic; Θ - optical property - integral oscillator strength; I – topological index of molecular structure; C_0, C_1, C_2, D_0, D_1 , D_2– empirically determined coefficients.

References

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