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Opinion

Chemical Mesoscopics for the Mesoparticles Reactivity Explanation

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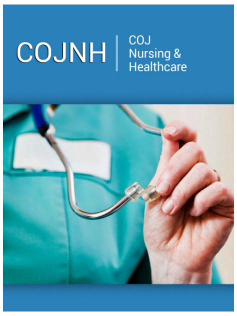
ISSN: 2577-2007



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Submission: December 8, 2020

Published: January 28, 2021

Volume 7 - Issue 1

How to cite this article: Kodolov Vladimir, Kodolova Chukhontseva VV. Chemical Mesoscopics for the Mesoparticles Reactivity Explanation. COJ Nurse Healthcare. 7(1). COJNH. 000651. 2021. DOI: 10.31031/COJNH.2021.07.000651

Opinion

The Chemical Mesoscopics is the scientific trend studied the mesoscopic systems reactivity at the beginning of formation and at further active behavior in media and in materials. The theoretical basis of this trend gives the explanation for peculiarities of nanostructures formation including reaction within nanosized reactors as well as the behavior of minute quantities of them in media and materials with properties change of latest.

The fundamental postulates of Chemical mesoscopics, according to which

a) regulated mesoscopic system must be many much little than macro system which is found in contact with it, b) the charges (negative and positive) quantization is observed, d) such phenomena as interference with chemical bonds and also annihilation with the creation of radiation and direct electromagnetic fields, that stimulate the electron shift in high energetically region.

Chemical mesoscopics is also based on the notions about self-organization and self-similarity [1]. According to the fractal theory [1] any system can be presented as aggregate of elements similar to whole system. These elements have own energetic and geometric (volume) parameters owing to which they are found within the system. The change of these parameters because of the action of external factors leads to disturbance of system balance. At this case the system is destructed or transformed. The estimation of these changes is possible with the using of the relative parameters in which the energetic and volume values are compared with the definite standard values for the correspondent elements (fragments) in the definite reaction series. This approach to reactivity consideration is near to Taft and Pal'm theoretical works [2]. For the relative energetic parameters the following formula $(\varepsilon-\varepsilon_0)/\varepsilon_0$ is proposed [3], where ε_0 corresponds to the surface energy for standard chemical fragment. In turn, analogous relative parameters are proposed [4] for the volume characteristics $(V-V_0)/V_0$.

The development of Chemical Mesoscopics in this direction is connected with the research of the size and energetic characteristics of chemical particles. The size of mesoparticles is denoted as approximately 10 nm, and the motion freedom of nanostructures (mesoparticles) is limited by the vibration with high frequency and electron transport across them. The peculiarities of mesoparticles consist in the radiation of energy quants of negative or positive charges. This radiation is the main reason of the stimulation of chemical processes. At the imposition of the negative charge quants the interference takes place and the chemical bonds are formed. In turn the imposition of the negative and positive quants together the phenomenon of annihilation is created. At this case the direct electromagnetic field is appeared that leads to the stimulation of negative charge quants moving and the growth of chemical bonds formation. The phenomena of interference and annihilation are reasons of start for self-organization process with reservation conformation order, which determine the finished product structure. For the process explanation the equation of Kolmogorov-Avrami [1] can be used -

$W = 1 - \exp(-k\tau^n)$, (1)

Where,

W - The part of obtained product (for instance, polymer),

k - the process rate constant,

τ - the duration of process,

n - the fractal dimension (for one measured process n = 1)

For the comparative estimation of reagents (or nanostructures) in one reaction series it's possible the application of the theory of free energy linear dependences. In this case the reactions are considered with using one of reagent as the standard compound for which W is fixed W_0. The estimation of reactivity can be proposed on the difference $W-W_0$, where W is calculated on formula 2, and W_0 is defined on analogous formula with changes $k_0\tau_0^n$. It's noted, the fractal dimension n do not change because the comparison is carried out for one type of reactions. The following equation for difference $W - W_0$ can be written –

$W - W_0 = \exp(-k_0\tau_0) - \exp(-k\tau^n)$, (2)

and after equation 2 transformation -

$W_0 = k/k_0(\tau/\tau_0)^n - 1$ (3)

If $\lg k/k_0$ is defined as -

$\lg k/k_0 = -2{,}3\ RT\{[(\varepsilon_0 - \varepsilon)/\varepsilon_0]a + [(V_0 - V)/V_0]b\}$, (4)

and then this expression after transformation stand in the equation 3, than the equation 5 is received -

$\lg (W - W0) = (\tau/\tau_0)^n \exp \{[(\varepsilon_0 - \varepsilon)/\varepsilon_0]a + [(V_0 - V)/V_0]b\}$, (5)

Where values a and b - parameters, which correct the influence polar and steric (spaced) effects on reactivity in polymerization, the relation $(\varepsilon_0 - \varepsilon)/\varepsilon_0$ [3,4]. correspondents to Taft constant σ (polarity constant), and the relation $(V_0 - V)/V_0$ - Taft constant E_s (steric or spaced constant) [3].

The application of above notions for the Chemical Mesoscopics development is very perspective because stimulates the mathematic apparatus creation for the chemical processes flowing direction prediction.

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