

CHAPTER 6

Bondonic Theory

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6.1 DEFINITION

The bondons describe chemical particles, which are associated with electrons implicated in the chemical bond, as single, delocalized, or lone pair; they have orientated direction of movement and depend on a chemical field. Another definition states that the bondon is a quantum particle, which is correspondent to the effect or distribution of superimposed electronic pairing in chemical bonds, having a behavior similar with a neutrino in mass, with a photon in velocity and with an electron in charge. For a nanosystem, it presents an observable lifetime at the fem to second level and a chemical bonding at an order of hundred Å and thousands of kcal/mol. The bondons can be found on the wave functions, on the covalent bonds, in dispersive-weak interactions (as in the ADN), on the mechanism of action between ligand and receptor, and even on the ionic interactions.

6.2 HISTORICAL ORIGIN(S)

The first attempt (Putz and Ori, 2015) in describing the chemical bonding belongs to Lewis (1916) who proposes a cubic model as representing the

atoms in the molecule and develops the octet rule. A couple of years later, Langmuir (1919) developed the hypovalent (such as BF_3) and hypervalent (such as PF_5) molecules which represent the basis of the double quartet theory of Linnett (1961). Later, starting from octet and the electron pairing rules specific in bonding was first developed the intuitive valence shell electron pair repulsion (VESPR) model (Gillespie and Popelier, 2001) and later the electron localization function (ELF) model (Becke and Edgecombe, 1990; Putz, 2005). In order to understand the chemical bonding from the quantum perspective, Putz (2010, 2012a) propose the so-called *bondon* as a quasi-particle which correspond to the chemical field of bonding, as a new boson to represent the chemical bond (Putz and Ori, 2015).

6.3 NANO-SCIENTIFIC DEVELOPMENT(S)

In his work, Putz (2012a) developed an algorithm in 15 steps (Putz, 2010, 2012a, 2012b). In the beginning, in the *first step*, one can start with the quantum Schrodinger equation of motion for which the Broglie/Bohm electronic wave-function can be defined as (de Broglie, 1923, 1925, 1953, 1954):

$$\Psi_0(t, x) = R(t, x) \exp\left(i \frac{S(t, x)}{\hbar}\right) \quad (1)$$

where S represents the phase action factor and R represents the amplitude, and in terms of the total energy E , the electronic density ρ and the momentum p have the formulas (Putz, 2012a):

$$R(t, x) = \sqrt{\Psi_0(t, x)^2} = \rho^{1/2}(x) \quad (2)$$

$$S(t, x) = px - Et \quad (3)$$

The *second step* (Putz, 2012a) assumes to verify the charge current conservation law recovery, which is responsible with electronic fields' circulatory nature, as in equality:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \quad (4)$$

In the *third step* (Putz, 2012a), the quantum potential V_{qua} can be recognized, if appears, along with its correspondent equation:

$$V_{\text{qua}} = \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \quad (5)$$

The electronic wave function is depicted in *step four* (Putz, 2012a), in term of the chemical field \aleph , as follows:

$$\Psi_G(t, x) = \Psi_0(t, x) \exp\left(\frac{i}{\hbar} \frac{e}{c} \aleph(t, x)\right) \quad (6)$$

with e the standard abbreviation with the formula:

$$e = e_0^2 / 4\pi\epsilon_0 \quad (7)$$

Starting from the following chain equivalence:

$$\aleph_{\#} \sim \frac{\text{energy} \times \text{distance}}{\text{charge}} \sim \frac{\left(\text{charge} \times \frac{\text{potential}}{\text{difference}}\right) \times \text{distance}}{\text{charge}} \sim \left(\frac{\text{potential}}{\text{difference}}\right) \times \text{distance} \quad (8)$$

one can express the bondons, carried by the chemical bonding field along the distance of bonding, having $\hbar c/e$ as the unit quanta. In *step five*, one can separate the terms with imaginary and real \aleph chemical field in order to rewrite the equation of wave-function with the group object (Ψ_G). The chemical field charge current is identified in *step six*, which is the term in the context of the transformation group. For the Broglie-Bohm wave function, Ψ_0 from the Steps (1)–(3) one need to establish, in *step seven*, the global/local gauge transformations which is similar to it and in *step eight*, on the pattern quantum equation is imposed an invariant condition for the wave function Ψ_G . Next, the \aleph chemical field equations are established (*step nine*), and the chemical field system is solved (*step ten*). The chemical bond at equilibrium is depicted in *step eleven* by assessing the stationary chemical field as follow (Putz, 2012a):

$$\frac{\partial \aleph}{\partial t} \equiv \partial_t \aleph = 0 \quad (9)$$

Along the bonding distance one can identify, in *step twelve*, the manifested Bondonic chemical field, noted with \aleph_{bondon} . After that, *step thirteen*, the possible flux condition of Bader is verified within the vanishing chemical bonding field (Putz, 2012; Bader, 1990), as follows:

$$\aleph_{\#} = 0 \Leftrightarrow \nabla \rho = 0 \quad (10)$$

In *step fourteen* (Putz, 2012a), the velocity of electrons in bonding is obtained by the Heisenberg relation of time-energy relaxation-saturation through their kinetic energy:

$$v = \sqrt{\frac{2T}{m}} \sim \sqrt{\frac{2}{m} \frac{\hbar}{t}} \quad (11)$$

The bondons' mass is determined in step fifteen by equating the Bondonic chemical field along with the chemical field quanta \aleph_0 , and the following equality is obtained (Putz, 2012):

$$\aleph_B(m_B) = \aleph_0 \quad (12)$$

By knowing the mass and velocity values for bondon, one can indicate, in general, which is the electronic behavior in bonding with the possibility of determining, in particular, the exact type of bonding (Putz et al., 2015). In order to predict, in the ground state, which are the values of energy and length necessary for a bondon to reach the unity of mass or its electronic charge (Putz, 2010, 2012a, 2012c, 2012d, 2012e), one needs to employ the following equations:

$$\zeta_m = \frac{m_B}{m_0} = \frac{87.8603}{(E_{bond} [kcal / mol])(X_{bond} [\text{Å}])^2} \quad (13)$$

$$\zeta_e = \frac{e_B}{e} \sim \frac{1}{32\pi} \frac{(E_{bond} [kcal / mol])(X_{bond} [\text{Å}])}{\sqrt{3.27817 \times 10^3}} \quad (14)$$

Results shows that, in the case of common chemical bonds, there is a small probability that the bondon will have the same charge as the electron, due to the fact that lower binding energy can span a longer distance having the same unit charge of electron and in the same time, being transmitted with the same relativistic velocity, phenomena also known as zitterbewegung.

6.4 NANO-CHEMICAL APPLICATION(S)

The link between the behavior of elements in the extended nanosystems such graphite layers and the macroscopic observable quantities can be realized with the aid of bondon. In this context, the bondon can be defined as the bosonic counterpart of the wave function of the bonding electrons (Putz, 2010, 2012a). In the ground state, the bondonic mass related with bond energy and length has the following form (Putz and Ori, 2012):

$$M_B = \frac{\hbar^2}{2E_{bond} X_{bond}^2} \quad (15)$$

For extended bonding systems, there is available an interdependency constraint of the Heisenberg type:

$$E_{bond} [kcal / mol] X_{bond} [\text{Å}] = \alpha, \alpha = 182,019 \quad (16)$$

By taking into consideration the previous formula (Eq. 16) one can obtain, for a nanosystem with hundred atoms and the energy of about 1000 kcal/mol, the value of 182.019 Å will be the spanned maximum bonding. This value can be also detected for a nanotube with the length equal with 18 nm across its end. In the same time, the bosonic condensation of bondons determines a bonding system to support along 100 Å, for example, along with a nanotube of 10 nm length, which is maximum of 1820 kcal/mol (Putz and Ori, 2012).

Due to the fact that, at the quantitative and qualitative description, the bondons support nonlocality spreading, one can be able to study the bondonic properties at extended systems, with further applications in nanomaterials engineering, e.g., silicone as nanostructure used in hydrogen storage (Putz and Ori, 2012; Jose and Datta, 2011).

In this context, the total bonding energy can be expressed as a sum of the thermal energy considered as bondon kinetic motion along with the topological contribution which describes the nanostructure physical information (Putz and Ori, 2012). The working equation is of the form:

$$\begin{aligned} \langle E_{Bond} \rangle [kcal / mol] &= - \frac{\partial \ln z_B^{[0]}(\beta, E_{Bond})}{\partial \beta} \\ &= \frac{1}{2\beta} + \Xi = \begin{cases} \Xi, \dots \beta \rightarrow \infty (T \rightarrow 0K) \\ \infty, \dots \beta \rightarrow 0 (T \rightarrow \infty K) \end{cases} \end{aligned} \quad (17)$$

With the specification that, i.e., there is a correspondence $V(x) \rightarrow \Xi$, i.e., for the periodic cell, there is a correspondence between driving potential and the topological descriptors.

In their work, Putz and Ori (2012) describe which is the role played by bondons in formation of Stone-Wales (SW) defects on the graphene fragments (e.g., defect-defect interactions and boundary conditions) using in this study only connectivity topological data to express specifically physical information instead of considering the density of the electronic distribution of the system. Defective hybrid nanoribbons systems were confirmed by first principle calculations (Dutta, 2009), with a single central SW defect in each super-cell, obtained after one diagonal bond is rotated in the net (Putz and Ori, 2012).

6.5 MULTI-/TRANS-DISCIPLINARY CONNECTION(S)

For a given system, the spontaneous symmetry breaking (SSB) determines its stable state to tend towards a different configuration which is characterized by the fact that possesses a lower symmetry than its Hamiltonian or Lagrangian symmetry correspondent, this characteristic being applied for both quantum and classical structures. The SSB method can be used in different types of theoretical Physics subjects, especially in modeling physicochemical phenomena. In honeycomb systems, the SSB effect determines the gap formation in the fermionic spectra (Araki, 2011), which is a similar phenomenon with the spontaneous break of the chiral symmetry from the theory of the strong coupling relativistic field. The SSB mechanism, same as the Higgs-like model states, is able to produce massive bosonic particle which can be used, in quantum systems, to mold the physical behavior. In their work, Putz and Ori (2015a) propose an original SSB algorithm designated to produce a certain type of Goldstone particles, i.e., with a mass related to the mass obtained by considering together all the electrons participating in the chemical bond. Apart from their typical occurrence, by symmetry breaking of the Lagrangian in terms of components of the chemical field, these Goldstone bosons can also be identified using the bondons, known as the quanta of the chemical bonding field (Putz, 2010, 2012a). This approach proposes the Goldstone symmetry breaking (GSB) mechanism as a method to obtain the general law of electronic and bondonic masses, applied to a set of several benzenoids for which their bondonic mass values were determined. For the bondonic mass, there are two topological descriptors used to construct its analytical expression: the sphericity (topological efficiency) index, noted with ρ , and the E -sphericity (extreme topological efficiency) index, noted with ρ^E . Starting from these considerate, one can define, first, the Lagrangian of the Schrodinger field (ϕ) which is produced by the potential V as the main index of the GSB algorithm, following the formula:

$$L = i\hbar\phi^*\dot{\phi} - \frac{\hbar^2}{2m_0}(\nabla\phi^*)(\nabla\phi) - V\phi^*\phi \quad (18)$$

Using the ρ and ρ^E indices, one can also express the relationship between the potential ϕ^4 and the chemical field which is rooted in the chemical reactive/valence energy parabolic expression (Parr and Yang, 1989; Putz, 2011) as follow:

$$V(\phi) = -\rho\phi^2 + \frac{1}{2}\rho^E\phi^4 \quad (19)$$

After several mathematical artifices, the chemical bonding field (ϕ) is given by the solution of the following differential equation:

$$i\hbar\dot{\phi} = 3\rho^E\phi^5 + \frac{15}{2}\rho\sqrt{\frac{\rho^E}{\rho}}\phi^4 + 6\rho\phi^3 + \frac{3\rho^2}{2\rho^E}\sqrt{\frac{\rho^E}{\rho}}\phi^2 - \frac{\rho^2}{\rho^E}\phi - \frac{\rho^3}{2(\rho^E)^2}\sqrt{\frac{\rho^E}{\rho}} \quad (20)$$

Considering the Hartree's atomic unit of energy of the form $Ha = 27.11$ eV, the spontaneous breaking symmetry bonding field can be rewritten in the expanded form of the first order:

$$\phi_B = \phi_\infty \left[1 + 6Ha\beta \left(\frac{1}{2}\rho^E\phi_\infty^4 \right) \right] \quad (21)$$

The bondonic field can also be expressed in a simpler manner, as depending only on the length of the chemical field action, the E -sphericity and with the temperature considered an intensive physical parameter, with the expression:

$$\phi_B = e^{-\frac{r}{a_0}\sqrt{2\rho^E}} \left[1 + 3\beta\rho^E e^{-4\frac{r}{a_0}\sqrt{2\rho^E}} \right] \quad (22)$$

In the same manner, the bondonic mass can be determined to start from the expression:

$$m_B = \frac{m_0}{a_0} \int_0^\xi |\phi_B|^2 dr \quad (23)$$

with obtaining its integrated form:

$$\begin{aligned} m_B &= \frac{m_0}{a_0} \int_0^\xi e^{-2\frac{r}{a_0}\sqrt{2\rho^E}} \left[1 + 3\beta\rho^E e^{-4\frac{r}{a_0}\sqrt{2\rho^E}} \right]^2 dr \quad (24) \\ &= \frac{m_0}{10\sqrt{2\rho^E}} \left[5 \left(1 - e^{-2\frac{\xi}{a_0}\sqrt{2\rho^E}} \right) + 10Ha\beta\rho^E \left(1 - e^{-6\frac{\xi}{a_0}\sqrt{2\rho^E}} \right) + 9(Ha)^2 \beta^2 (\rho^E)^2 \left(1 - e^{-10\frac{\xi}{a_0}\sqrt{2\rho^E}} \right) \right] \end{aligned}$$

Applied to a set of polycyclic aromatic hydrocarbons (PAH) molecules, the results show that the bondons are formed in molecules with $\rho \neq 0$, the first carbon bond creation determining a mass value closed to maximum. After that (the presence of first C-C bond) the sphericity become the one that is influencing the bondonic mass. There was also determined a relation between the aromaticity character and the bondonic mass, i.e., a highly

aromatic molecule will present a higher value for the bondonic mass (Putz and Ori, 2015a).

6.6 OPEN ISSUES

There were many questions raised by the bondon, as a new concept in physical science, such as which is the maximum distance which can be considered a bond between two atoms, or what is exactly the bonding manifestation between to atoms (Putz and Tudoran, 2014). On the other hand, the next frontier in nanoscience appears to be the entangled chemistry on graphene, already predicted by Putz and Ori in their work (2015b), which will make possible the synthesis, control and molecular design on the graphene pattern and even the chemical bonding teleportation. In order to achieve these tasks, one will need to control first the transformation boson-fermion, at a large scale, and then, at the chemical bonding level, the wave-particle quantum symmetry breaking should also be controlled. Due to the fact that the quantum mechanics' principles can be used to describe unitary the condensation, delocalization and long-range phenomena, the bondonic chemistry becomes, in this context, an appropriate conceptual method for this type of research.

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KEYWORDS

- **bondon**
- **boson**
- **fermion**
- **goldstone symmetry breaking**
- **spontaneous symmetry breaking**
- **wave function**

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