


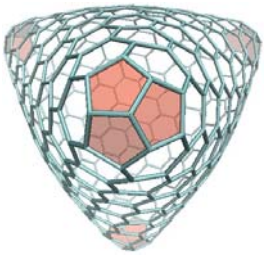

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SYNTHESIS PAPER

entitled

QUANTIFICATION OF THE CHEMICAL BOND WITHIN ORTHOGONAL SPACES OF REACTIVITY. APPLICATIONS ON MOLECULES OF BIO-, ECO- AND PHARMACO-LOGICAL INTEREST

including the work done and the results obtained in relation to the objectives achieved during the research grant

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on year 2013.

Abstract

The 2013 research phase, and the last one of this present grant continued the „bosonic" approach of matter and the chemical bonding as a quantum condensate, based on the electronic bosonation in chemical bond with formation of the quantum particle (the bondons) driving the chemical bond force, innovatively developed in the previous phases of the project, 2010-2012; however, the present approach is focused on quantum modeling of chemical reactivity in explaining the reactivity mechanisms of molecules and of the nanocomposites, eventually based on the bosonic – bondonic phenomenology; besides, it is also realized the topological and algebraic description of the chemical – biological interaction and toxicity by applying the variational type models for a better understanding and control of ligand – receptor binding action, with frontier applications in functional medicine.

Goals and Results

1. The quantum-orthogonal modeling for chemical bonding at the atoms-in-molecules level: bosonation by bondons and the associate nanosystemics properties (papers [1- 11]).

In the effort of unifying the chemical reactivity principles of electronegativity and chemical hardness, the electrophilicity index (ELFIL) appears as a unification-natural measure of the first two electronic complementary tendencies. Moreover, due to the inverse dependence of the ELFIL with the global chemical hardness it opens the door of being evaluated within the method of chemical softness, with all of the principle and methods available on the Density Functional Theory (DFT). In this context, the present work allow the introduction of the local and kernel electrophilicities based on long-range local and kernel softness, respectively, with fulfilling the main hierarchical bilocal-local-global constraints by successive integration rules, symmetry, all of them with conceptual consistency. The obtained bilocal expression (Figure 1) is original and general, not being limited by the knowledge of the functional dependence, of the electrons number from system (or the valence ones) E(N) and therefore not being affected by the discontinuity in energy-charge transfers (derivatives) as earlier formulations from literature were shown. Instead, the present approach is based exclusively to density and external applied potential dependence, as long as it is implemented a bilocal structure the kernel chemical softness, on the atoms and molecules, and moving forward, as implied in chemical phenomena. A numerical illustration is realized by calculation and the atomic scale representation associate to behavior, by softness kernel, on the valence electrons

for the principal groups and periods (Figure 1), being remarkable the respecting of the hierarchies already described by electronegativity, especially for the halogens and alkaline metals systems. The method and the chemical bilocal information of the electrophilicity can be successfully applied even on the extended electronic systems level of the nanosystems type, with bondonic and distance interaction effects included.

Figure 1. Bi-local electrophilicity index, in analytically and graphical analysis for elementary atomic systems [1].

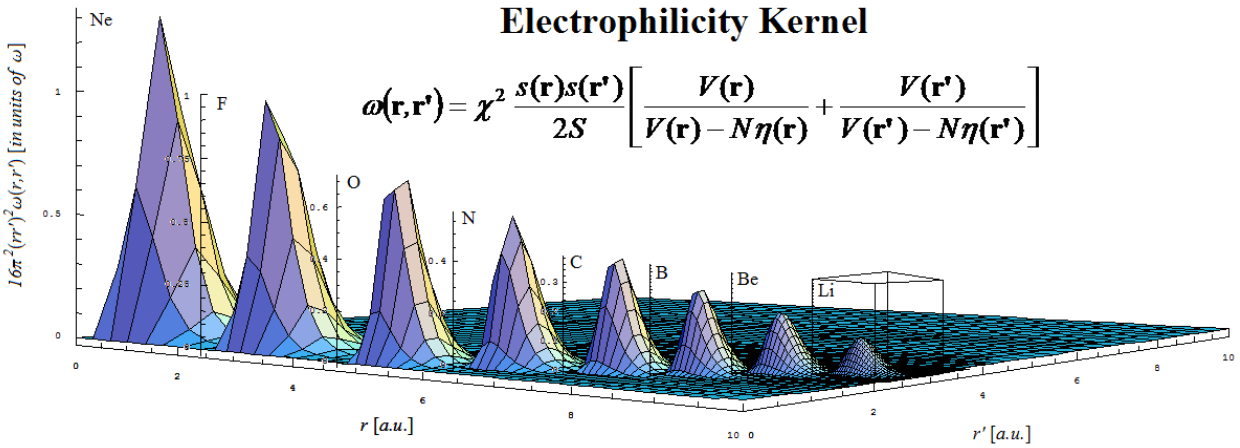
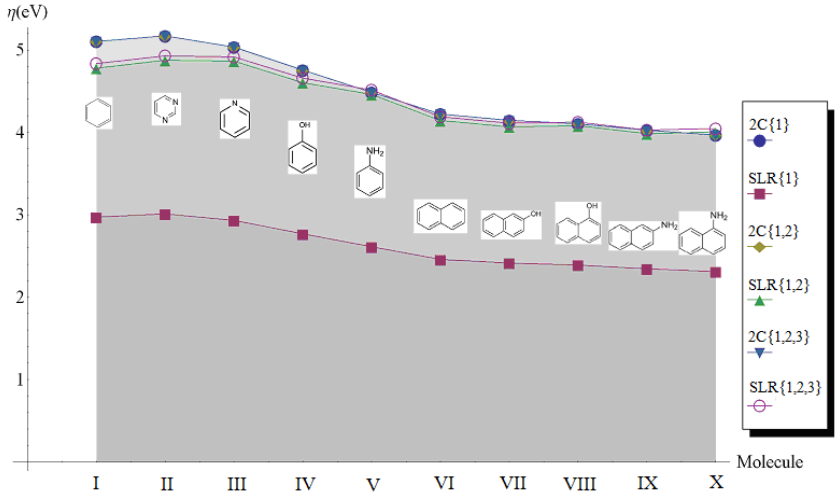


Figure 2. Chemical hardness representation for a representative organic molecular set, calculated with the central finite differences methods (2C) along that with spectral type resolution (SLR), involved in electronic exchanges with associate successive valence levels (1,2,3), HOMO(highest occupied molecular orbital)-LUMO (lowest unoccupied molecular orbital) [3].



On the other hand, in relation with the chemical hardness influence in electrophilicity and chemical exchange of atoms-in-molecules, involved in the inter-molecular interaction, and for the extended systems reactivity (nanosystems), Koopmans' theorem is analyzed on three approximation platforms, this way clarifying: (i) the orbital energy behavior as being natural *repositioned* from their eigen- or Flock space (of the quantum occupancy) when the numerical implementation is made by the associate wave-functions' *Hilbert-Banach basis set–this being the most subtle aspect of analysis, because it "saves" the TK validity by the dichotomy of "numeric-observed" effect towards the "proper-itself" from the quantum prediction;* (ii) the "frozen spin-orbitals" of the involved levels in extracting or adding of electrons in an individual (affinity and ionization) chemical processes; (iii) the most severe approximation by

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generalization of the second one to superior orders of electronic affinity and ionization (from HOMO and LUMO levels successively), with promising results (Figure 2) for its validity, with further applications in nanochemical systems.

2. The variational-orthogonal modeling of chemical bonding at the ligand-receptor interaction level by biological and ecotoxicological structure-activity relationship (papers [12-17]).

Discovering and validating new drugs and their active molecules involves a complex and lengthy, however a fascinating journey. Fortunately, there are several strategies to accelerate the selection of candidate substances for future medicine, among them, quantitative structure-activity relationship aka QSAR (and QSPR: quantitative structure-property relationship) methods furnish the analytical framework in which the mechanism of biological activity may be unfolded with appropriate conceptual algorithm for selecting and interpreting the computational implementation and statistical results. The present work advances such a coherent computational-conceptual algorithm for better understanding of chemical-biological interaction, through applying it towards better understanding of drug-HIV interaction mechanism (here 1,3-disubstituted uracil based type) "chemical untied" (represent by the SMILES molecule-Simplified Molecular-Input Line-Entry System, initially with exclusively computational value, but assumed here also at the conceptual-dynamic level in interaction) in the way of electrons' pairing depleting (i.e. the chemical bond) by the lipophilic pass (viz. electrophilic) by the cell wall (here HIV) in the form of ligand-in-situ projection, nearer the spatial conformation of the molecular "pocket" on the receptor level (Figure 3). This SMILES framework it can be used in QSAR screening for predictive molecular set by means of best correlations descriptors, especially with their hierarchy in bio/eco/pharmacologic action, in the orthogonal space of chemical reactivity descriptors of electronegativity (χ) and chemical hardness (η) along the mixed reactivity indices as chemical power (π), electrophilicity (ω); for all these there are meaningful optimum principles as the electronegativity adducts' equalization, or the maximum of chemical hardness in reactivity stable products. Specifically, for the mechanistic approach present by QSAR modeling of chemical-biological interaction explicitly assumes and implements *variational principles* in complementary forms, explaining the dynamic of the specific interaction, namely:

- By considering SMILES counterpart of envisaged molecules, *longest* SMILES molecular chain (LoSMoC) used in pre-selection of the target molecular set form QSAR analysis;
- By considering the descriptors in the orthogonal chemical reactivity space for which exists *min-max* prescription in evolution analysis (reported at reaction coordinate, solubility, topology, etc.);
- By selecting the *highest* QSAR correlation among SMILES screening based compounds;
- By employing the transitivity of the QSAR descriptors, as a manifestation of the *close up* of the molecular physicochemical properties, in extracting from endpoint's chains the structural causal hierarchy bio/eco/pharmacologic manifested;
- By ordering the multi-descriptor dependencies with the help of *ordering* of local/mono-linear correlations, especially for establishing the triggering chemical causes of bio/eco/pharmacologic actions;
- By recognizing the restrained number of relevant correlation models on endpoints' paths through assuring the complete coverage of the considered Banach space of chemical reactivity descriptors by *smallest* number of highly rated correlations' dependencies;
- By performing the *least* path-length search along all possible correlation' combinations built on the selected models from previous step.

All together, these steps provide 7-fold variations ("*longest*", "*min-max*", "*highest*", "*close up*", "*ordering*", "*smallest*", and the "*least*") from a given pool of molecules with a recorded biological activity towards establishing the chemical mechanism of structural causes targeting the observed effect. Those steps were all integrated to the actual application having as the final result the mechanism by which selected uracil based pyrimidines produce anti-HIV action, in terms of comprehensible chemical stages (relating frontier charge transfer between involved ligand molecules and receptor) at the cell level; this way it is molded the ligand-receptor interaction through the SMILES transformed molecules projected on the receptor site.

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Figure 3. The mechanistic representation of the QSAR results for the virtual uracil compounds involved in HIV interaction by transforming the gas-phase molecule (ligand L) in SMILES stage, which are projected in the receptor site (R, on the V1/V2 leap of the gp120 region from HIV), based on the variational principles for the electronegativity (χ), chemical hardness (η), chemical power (π), and electrophilicity (ω) indices, along with lipophilicity (logP), through the HIV cell membranes: A) docking by the gp120 glycoprotein; B) transduction through the transmembranar gp41 glycoprotein; C) through lipidic membrane; D) through the cell matrix; E) through capsid; F) in RNA; all along to G) reverse transcriptase [12].

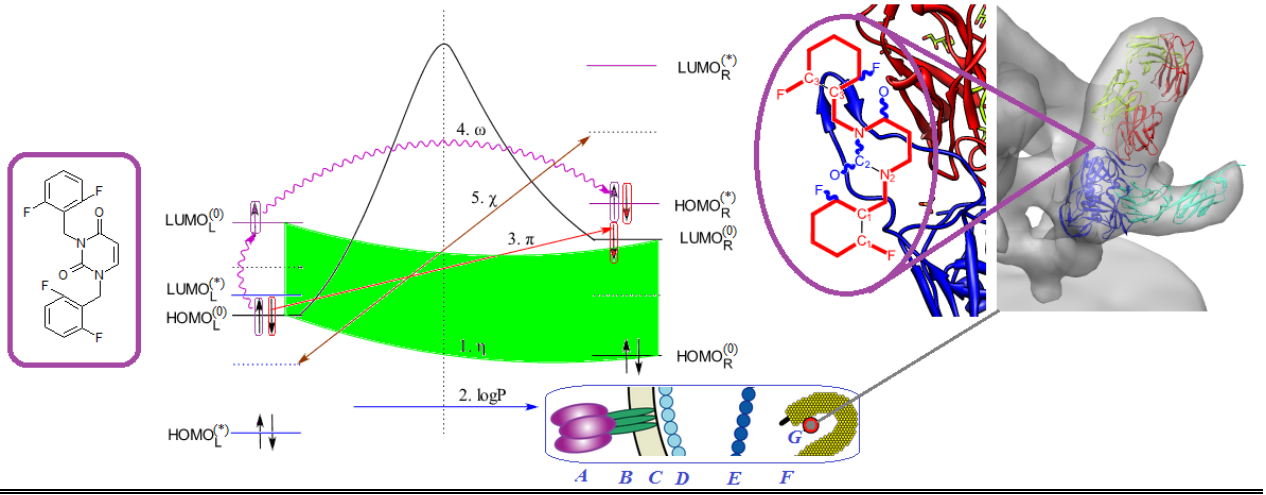
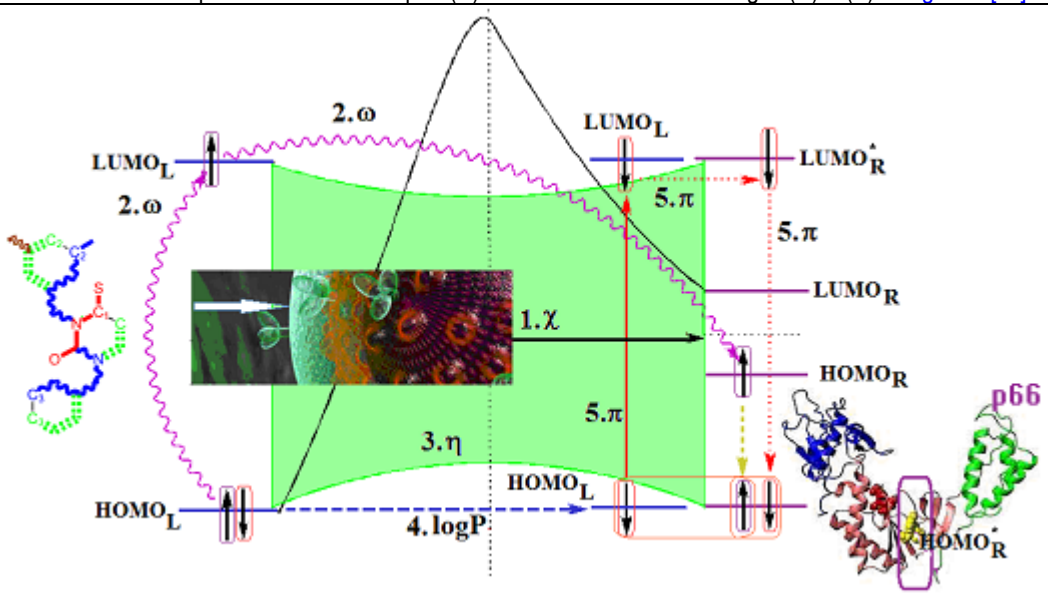


Figure 4. The mechanistic representation analysis of the molecular orbital interaction between the pyrimidine's uracil types derivates and HIV with the aid of the variational spectral-QSAR through the branching SMILES for the chemical bond of the ligand (L) projected on the "molecular pocket" form the receptor (R) for the cell transduction stages (D) & (E) in Figure 3 [13].



SMILES approach on the QSAR screening step and for generating the ligand-receptor interaction mechanism is further generalized by combining the *longest* SMILES molecular chain (LoSMoC) molecules with the branching SMILES (BraS) molecules, for whom, by the "competition" in the studied anti-HIV action it generates the complementary mechanism of Figure 4 for that one in Figure 3.The present approaches have a major contribution in formulating the "covalent bonding" in modeling of

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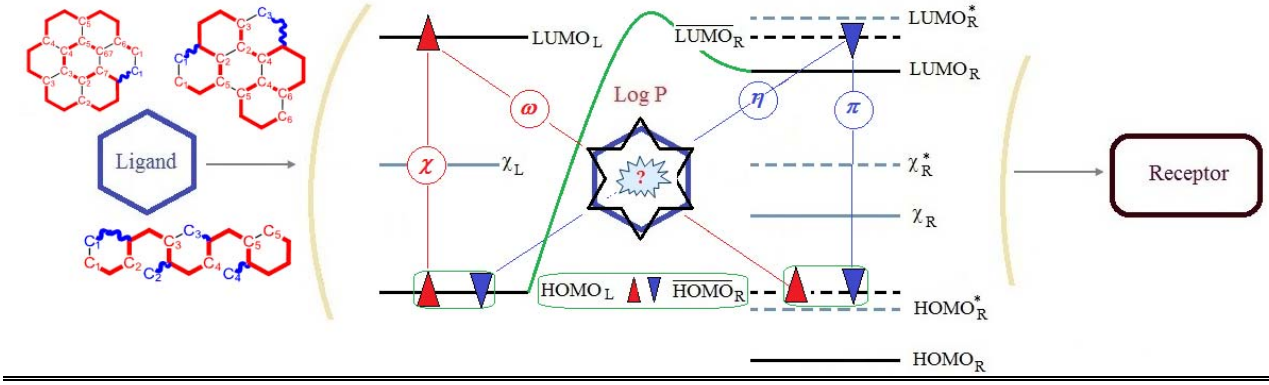
bio/eco/pharmacologic action, with large perspective of electrophilic theory generalization in order to understand and preventing the carginogenesis in special and the toxicity in general.

3. Topo-dynamic modeling of chemical bond in pharmacophore bonding, in multidimensional orthogonal space of reactivity (papers [18-22])

Finally, it arises the open issue regarding the degree with which this new type of approaching by SMILES is really functional and independent by the observed bio-eco-pharmacologic activities and by computational means operated. In this way, the present research considers also the lipophilicity correlated with the orthogonal space of chemical reactivity (electronegativity, chemical hardness, chemical power, electrophilicity) with genuine molecule (gas phase type) and respectively with their SMILES form (assumed specific in cellular environment), for a toxicants set of PAHs type (polycyclic aromatic hydrocarbons), Figure 5. The correlation results clearly revealed how the SMILES stage molecules became better correlated with the associated lipohilicity (in principle, for gas phase molecules, lipohilicity is a cell medium response form at the initial structural „pattern" of the „ingested" molecules in the bio-eco-pharmacologic medium). The investigation success allows a future approach of materials based on extended chemical structures (nanosystems and nanotubes types) in interaction and in kinetic/catalyses with the biological organisms, by prediction and laboratory (and even industrial) synthesis with pre-information structural correlated and/or optimized with the cellular environment targeted for the respective molecular "immerse" and interaction. This way, the present studies represent the base of systematic modeling with reactivity indices in the orthogonal space of electronic correlation form the bi-local, local and global level from chemical structures, by genuine chemical bond, but also decomposed (viz. SMILES) further engaged in macro-molecular iterations, or membrane transductions (lipohilicity) in cellular (crowded) environment, of high interest in present and future pharmacodynamics.

Figure 5. The representation of the ligand-receptor type interaction through the cell wall, "guide" by the lipophilic behavior of the molecular structures involved, correlated at its turn with the reactivity indices of electronegativity (χ), chemical hardness (η), which realize the equalization phase of the levels and energetic interval HOMO-LUMO, respectively, completed by the step of stabilizing the transfer of the electronic pair (chemical bond) between HOMO and LUMO levels of ligand and receptor, driven by the effect of electrophilicity (ω) and of chemical power (π) which quantify the activation energy necessary in bonding and in the maximum number of interchanged electrons, respectively – completing this way the "scenario" of the biologic/lipophilic activity by the effect of the chemical reactivity indices [18].



Conclusions and Perspecives

The 2013 stage, as the last one of this project accomplished, in synergic manner, essential conceptual and computational goals about the way that the reactivity and chemical bond influence and guide the bio/eco/pharmacologic activity, as follows:

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- The formulation of chemical reactivity hierarchy by the aid of the electrophilicity concept evaluated on the level and with *kernel,* local and global correlation for elementary atomic systems.
- Atomic correlation modeling in molecules (organic in special) with Koopmans and Hükel generalized theorems. The extended nanosystems characterization and carbon fragments with bondonic model of the chemical bonding.
- The explicit formulation on the *multi-variational steps* in *establishing* the chemical-bio/ecotoxicologial bonding mechanisms by structure-activity/toxicity correlations.
- Quantum basis establishing the topo-molecular bonding mechanism with biological receptors from environment.
- Chemical reactivity influencing and orthogonal space modeling of chemical reactivity driving ligand-receptor bonding with application in amino-acids and bio-eco inorganic and bio-eco organic fragments.
- Quantum bases and structural nanochemistry exploration: correlation of structure with the reactivity and lipophilicity properties, by statistics and classical algebras algorithms but also with the spectral-diagonal generalized approach, new proposed; application on the benzenoids compounds and on their pharmacologic effect in the context of protein-substrate interactions.

All in all, a unitary vision of the matter structure *involved* in chemical reactivity there was created, while unifying the principles of atomic and molecular interaction on the nanomatter level, by functional integration of the quantum particles evolution, a high perspective approach in order to unify the physical-chemical principles on the nanoscience level [23-25]. This way, the *unfolded studies* sustain the conceptual reconsidering of the matter structure's fundamental perspective, i.e. the photons, electrons, atoms, molecules, biomolecules, and nanosystems in reciprocal interaction, from the fundamental *in cerebro-in silico* perspective. The *accomplished* predictions are constituted as an efficient way to improve both the quality in life welfare and for the natural resource exploitation for a sustainable "green" future. More than that the present researches simulate, predict and explore new phenomena which are pursuit by adaptive and functional control, and which can consist as the basis for new principles and applied-recycling technologies integrated within the "life polynomial": *human knowledge – production/social utility – economy of resources – design of environment interaction – nature equilibrium*, as it will be continued in the next phases of complex scientific investigation of natural (chemo-bio-physical) systems from the next programs of European research leg and funding, at horizon 2014-2020!

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