Chapter 5

Nanoroots of Quantum Chemistry:
Atomic Radii, Periodic Behavior, and Bondons

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ABSTRACT

This chapter identifies specific roots of chemistry and quantum chemistry and advances the idea that length and energy carry major roles at the nano-quantum level. A detailed exposition of this binom is unfolded under the specific radii-electronegativity or radii-chemical hardness that is then naturally extended to the radii-chemical descriptors relationships, having the atomic periodicity as the main benchmark check for their reliability. As such, considering different analytic electronegativity scales, they are reported and compared to the respective atomic orbital radii scales, both for the electronic density formulation, as uniform atomic electronic assembly, and for Slater type density orbital, respectively. The scheme for atomic orbital radii is further generalized by chemical descriptors in the frame of density functional theory. Finally, the chemical bond is treated through introducing the chemical quantum particle-the bondon-as a molecular nano-reality in modeling the energy-length space towards the chemical space, or bonding and reactivity. The existence of the chemical field along the associate bondon particle $\mathcal{B}$ characterized by its mass $(m_{\mathcal{B}})$, velocity $(v_{\mathcal{B}})$, charge $(e_{\mathcal{B}})$, and life-time $(t_{\mathcal{B}})$ are revealed by employing the combined Bohmian quantum formalism with the U(1) and SU(2) gauge transformations of the non-relativistic wave-function and the relativistic spinor, within the Schrödinger and Dirac quantum pictures of electronic motions.

1. INTRODUCTION

Other than the electronegativity concept, perhaps one of the most influential concepts in chemistry (Pauling, 1960; Mulliken, 1934; Gordy, 1946; Iczkowski & Margrave, 1961; Klopman, 1965; Hinze & Jaffe, 1962; Parr et al., 1978; Bartolotti et al., 1980; Bartolotti, 1987; van Genechten et al., 1987; Proft & Geerlings, 1997; Putz, 2003; Putz et al., 2003; Putz et al., 2005; Putz, 2006a; Putz, 2007; Putz, 2008a; Putz, 2009a; Putz, 2011a-c), there is a class of related objects that can properly define and describe the tendency of an electronic system (atomic herein) to attempt a chemical coordination. Such objects like (atomic) orbital radii (Ghosh & Biswas, 2002; Putz et al., 2003; Putz, 2004), polarizability (Ghanty & Ghosh, 1996; Hati & Datta, 1994; Putz, 2010a), hardness (Parr & Pearson, 1983; Robles & Bartolotti, 1984; Gázquez & Ortiz, 1984; Pearson, 1985; Pearson, 1997; Putz et al., 2004; Putz, 2006a; Putz, 2008a-b; Tarko & Putz, 2010), softness (Parr & Yang, 1989; Garza & Robles, 1993; Senet, 1997; Matito & Putz, 2011) and the Fukui function (Yang et al., 1984; Gázquez et al., 1987; Berkowitz, 1987; Senet, 1996; Ayers & Parr, 2000) are called the *chemical descriptors* because their capabilities to index the capacity of an electronic system to interact with another one in the chemical energy range (Kohn et al., 1996). Finding a suitable picture to compute these chemical descriptors in an analytical fashion will strongly contribute to depict the chemical reactions and transformations from a unitary point of view (Chermette, 1999; Putz, 2009b).

On the other side, the chemical bond, perhaps the greatest challenge in theoretical chemistry has generated many inspiring theses over the years, although none definitive (Lewis, 1916; Langmuir, 1919; Thomson, 1921; Heitler & London, 1927; Pauling, 1931a-c; Hückel, 1931; Doering & Detert, 1951; Parr & Yang, 1989; March, 1992; Bader, 1990; Bader, 1998; Mezey, 1993; Putz, 2008c-d; Putz, 2009c-d; Putz, 2010a; Putz, 2011d-e). Few

of the most preeminent regard the orbitalic based explanation of electronic pairing, in valence shells of atoms and molecules, rooted in the hybridization concept (Pauling, 1931c) then extended to the valence-shell electron-pair repulsion (VSEPR) (Gillespie, 1970). Alternatively, when electronic density is considered, the atoms-in-molecule paradigms were formulated through the geometrical partition of forces by Berlin (1951), or in terms of core, bonding, and lone-pair lodges by Daudel et al. (1983), or by the zero local flux in the gradient field of the density $\nabla \rho$ by Bader (1990, 1998), until the most recent employment of the chemical action functional in bonding (Putz, 2009c-d).

Yet, all these approaches do not depart significantly from the undulatory nature of electronic motion in bonding, either by direct wave-function consideration or through its probability information in electronic density manifestation (for that is still considered as a condensed—observable version—of the undulatory manifestation of electron).

In other words, while passing from the Lewis point-like ansatz to the undulatory modeling of electrons in bonding, the reverse passage was still missing in an analytical formulation. Only recently the first attempt was formulated, based on the broken-symmetry approach of the Schrödinger Lagrangean with the electronegativity-chemical hardness parabolic energy dependency, showing that a systematic quest for the creation of particles from the chemical bonding fields is possible (Putz, 2008d).

Following this line, the present work makes a step forward and considers the gauge transformation of the electronic wave-function and spinor over the de Broglie-Bohm augmented non-relativistic and relativistic quantum pictures of the Schrödinger and Dirac electronic (chemical) fields, respectively. As a consequence, the reality of the chemical field in bonding was proved in either framework, while providing the corresponding bondonic particle with the associate mass and velocity in a full quantization form. In fact, the Dirac bondon was found to be a natural generalization of

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