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The Rigged QED density interpretation of physical-chemical properties of molecules and chemical processes.

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The electronic energy density associated with electron density [1a,b] was used for real space representation of local physical-chemical properties of atoms and molecules. New interaction energy density, regional chemical potential and energy based bond orders were obtained on the frame of the same field theory that was used before for tensorial characterization of chemical bonds and atomic or molecular regions [1]. The stress tensor description of covalent bond formation via so called spindle structure, non-positively defined kinetic energy density and mechanical boundaries of atomic and molecular regions in shape of dynamical forces acting on electrons has already proved its usefulness in description of chemical processes [2]. This new concepts, all visualized in three-dimensional space, give very fresh and deep insight into the origin and effects of chemical and physical interactions and chemical reactivity.

In the stress tensor analysis, one can visualize the propagation of local force in real space by tracing the congruence of the principal axes, leading to the bond line as the envelope, as shown in Figure 1(a). The spindle structure accommodates a bundle of bond lines carrying tensile stress region in between a pair of compressive ones on the edges with a shape of bond if they connect a pair of R_D's. In Bader's analysis topologically defined bond paths, bond critical points and electron cloud enclosed regions serve as regions of space carrying the information about bonding interaction and atomic regions [3]. Rigged QED analysis at stationary point provides the chemical interaction characteristic with the Lagrange point $\vec{r}_{Lagrange}$ at which the tension (and also the Lorentz force) vanishes for electron to take a rest in course of the chemical bond, as shown in Figure1(b). We suggest that $\vec{r}_{Lagrange}$ carries heavy load of interaction information, however it may be not complete. The $\vec{r}_{Lagrange}$ are common for all molecules and easy to identify. According to I. Pregogine an open system at stationary state (with constant extensive quantities) organizes itself in a way to minimize total entropy production. The entropy production takes place at the boundaries, not within the system, where extensive properties are exchanged with neighborhood. Here reveals a nature of Lagrange point as the trade centre. In contrast to Bader's AIM analysis [3] the Rigged QED peculiar point is determined by dynamical forces acting on electrons thus has mechanical origin instead of being a topological parameter.

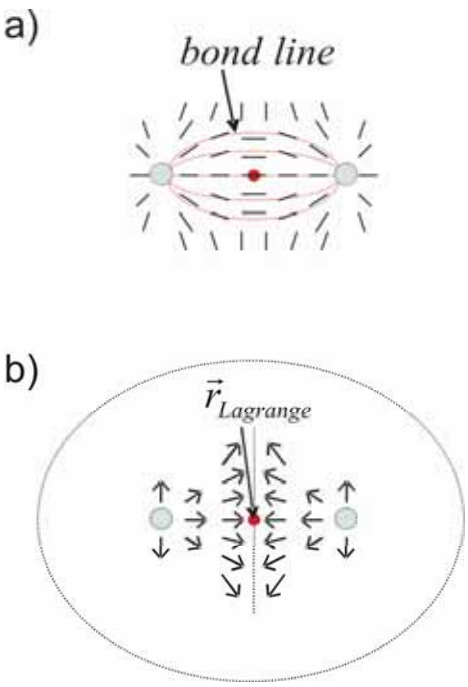

Figure 1. The bond lines and Lagrange point $\vec{r}_{Lagrange}$:
a) the eigenvectors of principal stress constitute the bond lines,
b) the cancellation of tension defines Lagrange point (situated on a bond line).

[1] (a) A. Tachibana, Theor. Chem. Acc. 102, 188-1999. (b) A. Tachibana, Int. J. Quantum Chem., Quantum Chem. Symp. 21, 181-1987. (c) A. Tachibana, Int. J. Quantum Chem. 57, 423-1996; A. Tachibana and R. G. Parr, *ibid.* 41, 527-1992. (d) A. Tachibana, K. Nakamura, K. Sakata, and T. Morisaki, Int. J. Quantum Chem. 74, 669-1999.

[2] (a) Tachibana A (2003) Field energy density in chemical reaction systems. In: Brändas E, Kryachko E (eds) Fundamental perspectives in quantum chemistry: a tribute to the memory of Per-Olov Löwdin, vol 2. Kluwer, Dordrecht, pp 211–239, (b) Tachibana A (2004) Int. J. Quantum Chem. 100:981–993

[3] R. F. W. Bader, Atoms in Molecules - A Quantum Theory, Oxford University Press, Oxford, 1990