Maximum Probability Domains

Guillaume Acke[1], Benoît Braïda[2], Patrick Bultinck[1], Ángel Martín Pendás[3]

1. Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 (S3), B9000 Ghent, Belgium
2. Laboratoire de Chimie Théorique, CNRS and UPMC Univ Paris 6, 4 place Jussieu, 75252 Paris, France
3. Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, 33006 Oviedo, Spain

The Lewis model of the chemical bond treats electrons as discrete pairs, localized in a certain region of space. On the other hand, the molecular orbital approach to quantum chemistry considers electrons as delocalized over the entire space. Many new ways to extract Lewis-structural information from the wave function have been suggested, providing links between quantum and traditional chemistry.

One of these novel approaches is the use of maximum probability domains (MPDs) [1][2]. This method statistically localizes electrons in domains, by determining those regions of 3D space for which the probability of finding a given number of electrons is maximal. This method has successfully been applied to interpret covalent and ionic bonding [3][4]. However, MPDs have not yet been characterized by other chemical descriptors, which leaves their links with other conceptual quantities ill described. Furthermore, MPDs obtained from current implementations suffer from numerical inaccuracy, which clouds their properties [5].

In this presentation, I will introduce the theory of MPDs, extend it with novel concepts and novel algorithms. I will show how this theory can be applied to a range of chemical phenomena, and how this interpretation can lead to increased chemical understanding.

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