

Natural Bonding Energy



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Abstract

In computational chemistry, Natural Bonding Orbitals (NBOs) are instrumental in elucidating chemical bonding mechanisms by scrutinizing electron density distribution and the sharing of electrons for bond formation. NBO theory facilitates the creation of localized orbitals from molecular orbitals, offering a more nuanced depiction of actual bonding interactions. These NBOs play a pivotal role in characterizing chemical bonding, offering insights beyond traditional molecular orbital theory. They assess factors such as polarity, hybridization, and delocalization, which are crucial for predicting spectroscopic features, reactivity, and bond strengths. Moreover, NBO theory seamlessly complements Lewis's electron-pair model and other bonding theories, bridging the gap between intricate physical principles and simpler models. Utilizing mathematical formulas, NBO methods interpret electronic wave-functions in terms of localized Lewis-like bonds, optimizing the conversion into one-center and two-center orbitals. Continuously evolving with improved search algorithms and expanded analysis options, these methods have become indispensable tools in modern chemistry for the precise prediction and comprehensive understanding of chemical behavior and molecular structure.

Keywords: Natural Bonding Orbitals; Natural Lewis Structure; Natural Atomic Orbitals; Atomic Natural Orbitals

Introduction

In computational chemistry, natural bonding orbitals (NBOs) are a theoretical concept that help to explain and comprehend chemical bonding in molecules [1]. They provide a distinct viewpoint on how electron density is distributed within molecules, especially with regard to the process of atoms sharing electrons to form bonds [2]. The foundation of NBO theory is the hypothesis that a set of localized orbitals that more accurately reflect the bonding interactions that actually take place within the molecule can be created by mathematically transforming the wave functions of molecular orbitals [3]. A group of mathematical techniques known as "natural bond orbital (NBO) methods" used to analyze electronic wave functions using the terminology of localized Lewis-like chemical bonds. These techniques translate molecular characteristics into a "natural Lewis's structure" (NLS) representation of the wave function, which is directly analogous to the basic Lewis dot diagram used in first-year chemistry classes [4]. Thus, a "Lewis" (L type) member of the entire orthonormal set of NBOs is associated with each one-center (1c) lone pair or two-center (2c) bond pair of the Lewis structure diagram, while

the remaining "non-Lewis" (NL type) NBOs describe residual resonance delocalization effects (departures from idealized L-type representation) [5]. Natural atomic orbitals (NAOs), a comprehensive orthonormal set for best characterizing the effective atom-like components in the molecular environment, are the fundamental characteristic that sets NBOs apart [6]. The NAOs $\{\theta_i(A)\}$ effectively decrease to the equivalent atomic natural orbitals (ANOs) of isolated atoms at large interatomic separations [7]. However, in a particular molecular environment, the NAOs reflect the chemical give and take of electronic interactions; they differ significantly from free-atom forms in terms of size and shape (e.g., altered diffuseness due to increased anionic or cationic character; angular deformations due to steric pressures of adjacent atoms) [8]. Molecular orbital theory, which explains how atomic orbitals combine to generate molecular orbitals, is the foundation for the concept of NBOs. Molecular orbitals are commonly represented in conventional molecular orbital theory as mathematical combinations of atomic orbitals [4], with electrons filling these molecular orbitals in accordance with quantum mechanical principles. However, NBO theory goes a step farther

than that. It uses a technique known as “natural atomic orbital analysis” to change these molecular orbitals into a set of localized orbitals that more closely match individual atoms’ atomic orbitals [9]. This change aids in clarifying the precise bonding relationships that exist between the atoms in the molecule. The nature of chemical bonds, including their strengths, directional preferences, and the extent of electron delocalization, can be better understood by the application of NBO analysis [10]. Chemists can more accurately predict the reactivity and characteristics of molecules and obtain a deeper knowledge of their electronic structure by analyzing the spatial distribution and energy of NBOs. Compared to conventional molecular orbital theory, one of the main benefits of NBO theory is its capacity to offer a more comprehensible and chemically meaningful explanation of molecular bonding [11]. Because of this, it’s a useful tool for deciphering intricate chemical structures, comprehending how reactions work, and creating new molecules with the appropriate characteristics [12]. In conclusion, natural bonding orbitals provide an effective framework for molecular analysis of chemical bonding, revealing important details about the electronic structure and characteristics of molecules. Chemists can improve theoretical and computational chemistry and gain a deeper understanding of chemical reactivity through NBO analysis [13].

Discussion

Lewis-like localized few-center orbitals, known as Natural Bond Orbitals (NBOs), are used to characterize chemical bonding (Scheiner, 2022). Complex molecules, such as those seen in biological systems and materials research, can have their bonding examined using NBOs (Glendening et al., 2023). Because they offer a more thorough and precise explanation of bonding than conventional molecular orbital theory, NBOs play a crucial role in chemical bonding [4]. The polarity, hybridization, and delocalization of chemical bonds can all be examined using NBOs. NBOs contribute to a more comprehensive understanding of chemical bonding, which can help guide the creation of novel compounds with particular features and uses (Takatsuka & Arasaki 2021). Additionally, the electronic structure of molecules has been studied using NBO theory, which has been used to predict spectroscopic features, reactivity, and bond strengths (Cioslowski & Strasburger, 2021). NBO theory has numerous applications and is highly significant in chemical research. By offering a more thorough and precise explanation of chemical bonding, NBO theory has grown to be a vital instrument for today’s chemistry, with important effects for a variety of chemical applications (Stone, 2017).

Lewis’s type and Valence bond descriptions of chemical bonding are frequently linked to Natural Bond Orbitals (NBOs). The chemical connection with two shared electrons was discovered by Gilbert Lewis in 1916, more than a century ago. While they don’t completely replace the electron-pair model, other ideas such ligand field theory, orbital symmetry principles, the Dewar–Chapt–Duncanson model, and valence-shell electron-

pair repulsion serve to supplement it. Various techniques that bridge the gap between the complicated physical principles of chemical bonding and the straightforward Lewis model have been developed in recent decades (Zhao et al. 2019). The phrase “natural bond orbital methods” describes a group of mathematical formulas for interpreting electronic wavefunctions expressed in terms of localized Lewis-like chemical bonds. A technique for optimally converting a given wave function into a localized form, which corresponds to the one-center (“lone pairs”) and two-center (“bonds”) orbitals, is the foundation of NBO analysis [4]. The concept is based on using the molecular density matrix to determine the “natural” one-particle orbitals of the atoms within a molecule (Glendening et al. 2023). Improved search algorithms and labeling conventions for a wider range of chemical species, new analysis options that significantly expand the range of chemical applications, and novel “link-free” interaction with host electronic structure systems are all provided by the natural bond orbital analysis program (Glendening et al. 2013). Fundamental bonding ideas can be computed with contemporary wavefunction technologies, including restricted and unconstrained HF, DFT, MPn, etc., owing to a suite of algorithms known as natural bond orbital (NBO) approaches (Schiffmann et al. 2022).

The basic ideas of a chemical bond, Lewis’s dot structures, hybridization, resonance, and contemporary wavefunctions are all crucially connected by NBO methods. NBO investigations of contemporary wavefunctions show bonding notions such as bond order, hybridization, bond type (covalent, ionic, dative, σ , π , 2c-2e, 3c-2e, 3c-4e, etc.), resonance, charge transfer, and steric (Glendening, 2012). The strength, stability, and reactivity of the bond can all be determined by employing NBO analysis to analyze chemical bonds (Kolb et al., 2023). For a more comprehensible and approachable interpretation of the computer solutions of chemical problems, natural bond orbital analysis serves as a computational tool (Weinhold et al. 2016). Precise assessments of electron densities are made possible by NBO methods. The basic ideas of a chemical bond, Lewis’s dot structures, hybridization, resonance, and existing wavefunctions are thus crucially connected by means of NBO approaches. The NBO analyses of contemporary wavefunctions disclose bonding concepts including bond order, hybridization, bond type (covalent, ionic, dative, σ , π , 2c-2e, 3c-2e, 3c-4e, etc.), resonance, charge transfer, and steric (Glendening, 2012).

Conclusion

Natural Bond Orbitals (NBOs) represent a pivotal theoretical framework in computational chemistry, elucidating complex chemical bonding within molecules by transforming molecular orbitals into localized forms. Their unique inclusion of natural atomic orbitals (NAOs) enables a detailed understanding of electronic interactions in specific molecular environments. Going beyond conventional models, NBOs enhance our comprehension of chemical bonding, bridging historical perspectives and modern theories, and guiding the development of novel compounds. Their

applications extend to predicting spectroscopic features, reactivity, and bond strengths, making NBOs indispensable in contemporary chemistry. Evolving with improved algorithms, NBO methods serve as a concise yet comprehensive computational tool, linking fundamental chemical concepts to precise assessments of electron densities and contributing to a deeper understanding of chemical structures and reactivity.

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