

The chemical bonding in H_2 , H_2O and NH_3 molecules: proposing a fuzzy-logic description of electron sharing, localization and bond character

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Abstract

Chemical bonding is commonly introduced through discrete categories: covalent versus ionic, bonding versus antibonding, localized versus delocalized, and polar versus nonpolar. These distinctions are useful, but the electronic structure of a molecule does not itself contain such binary labels. Electron density varies continuously in space, bond polarity is graded, and the same molecular state can be interpreted through several complementary theoretical languages. This article develops a fuzzy-logic framework for describing chemical bonding in H_2 , H_2O , and NH_3 . The central idea is to represent selected chemical attributes - bond formation, electron localization, polarity, and directional participation - through membership functions whose values range continuously from 0 to 1. In this view, a bond is not forced to be either present or absent; rather, an internuclear region may possess a high degree of bonding membership while other regions retain membership in alternative descriptions. The framework is applied first to H_2 as the simplest two-center covalent system, then to H_2O as a strongly polar two-bond molecule with a bent geometry, and finally to NH_3 as a three-bond system in which the nitrogen lone pair introduces an additional electronic domain. Fuzzy rules are proposed to connect electron-density descriptors, electronegativity difference, bond distance and angular information. The approach is not presented as a replacement for quantum mechanics. It is instead an interpretive layer that translates continuous quantum-chemical information into chemically meaningful linguistic statements. The resulting description provides a compact way to discuss why H_2 is naturally characterized as a nearly symmetric covalent bond, why O-H and N-H bonds possess different degrees of polarity, and why molecular geometry cannot be separated from the spatial distribution of electron density. It is shown that fuzzy logic functions could act as semantic layers between numerical electronic structure and chemical reasoning.

Keywords: fuzzy logic; chemical bonding; electron density; membership functions; chemical descriptors.

1. INTRODUCTION

The concept of the chemical bond sits at the center of chemistry, yet the bond itself is not a directly observable object in the same way that a macroscopic piece of matter is. Experiments and quantum-chemical calculations provide quantities such as energy, electron density, molecular geometry, vibrational frequencies, dipole moment, and response properties. Chemists then organize these quantities into concepts such as covalent bond, ionic contribution, lone pair, bond polarity, and electron sharing. These concepts are extraordinarily useful because they compress a complicated electronic structure into a language that supports prediction and explanation.

The difficulty becomes apparent when these concepts are treated as strictly binary. A bond is frequently described as covalent or ionic, polar or nonpolar, localized or delocalized. In real molecules, however, these properties generally vary continuously. H_2 provides the clearest example: the two hydrogen atoms have the same electronegativity, so the electron distribution is symmetric, but the molecular electron density still occupies a finite region between and around the nuclei. In H_2O , the O–H bonds are strongly polar, yet they remain covalent in the conventional chemical sense. In NH_3 , the N–H bonds are also polar, but the magnitude and spatial organization of the polarization differ from those in water. Moreover, the lone pair on nitrogen cannot be described simply as an additional bond or as something completely unrelated to the molecular electron distribution.

Fuzzy logic offers a natural mathematical language for this situation. Introduced by Zadeh [1,2] as a framework for reasoning with degrees of membership, fuzzy logic does not require a proposition to be exclusively true or false. A statement such as “the bond is strongly covalent” can be assigned a membership value between zero and one. Importantly, this is not a probability. The membership value expresses the degree to which a molecular state belongs to a chemically defined class.

The objective of this article is not to replace molecular orbital theory, valence-bond theory, density functional theory, or electron-density analysis. Instead, the objective is to construct an interpretive bridge between quantitative molecular data and qualitative chemical language. H_2 , H_2O , and NH_3 form a useful sequence: a homonuclear diatomic molecule, a bent polar molecule with two bonds and two lone pairs on oxygen, and a pyramidal molecule with three bonds and one lone pair on nitrogen.

2. THEORETICAL BASIS

2.1 Chemical bonding as a continuous electronic phenomenon

At the quantum-mechanical level, a molecular state is described by a wavefunction or, in density-based approaches, by an electron density $\rho(\mathbf{r})$. Electron density is a continuous scalar field in three-dimensional space. Chemical bonding is associated with changes in this field relative to suitable reference atoms, together with energetic stabilization and changes in nuclear arrangement. Consequently, a binary label such as “bond” is an interpretation imposed on continuous electronic information.

$$\rho(r) = N \int |\Psi(r, x_2, \dots, x_N)|^2 dx_2 \dots dx_N \quad (1)$$

A useful conceptual quantity is the density redistribution associated with bond formation. If $\rho_{\text{mol}}(r)$ is the molecular electron density and $\rho_{\text{ref}}(r)$ is a reference density assembled from separated atoms, one may define:

$$\Delta\rho(r) = \rho_{\text{mol}}(r) - \rho_{\text{ref}}(r) \quad (2)$$

The sign and magnitude of $\Delta\rho(r)$ indicate where electron density is accumulated or depleted relative to the selected reference. Because different reference states lead to different numerical redistributions, $\Delta\rho$ is best treated as a descriptor rather than an absolute definition of bonding.

2.2 Fuzzy sets and membership functions

In classical set theory, an element either belongs to a set or does not. A fuzzy set replaces the binary indicator with a membership function $\mu(x)$ satisfying $0 \leq \mu(x) \leq 1$. For a chemical property P , one can define a fuzzy set such as “strongly covalent bonds” and assign each bond a membership value according to selected molecular descriptors.

$$\mu_P(x): X \rightarrow [0,1] \quad (3)$$

A membership value should not be confused with a probability. A value of 0.80 does not mean an 80% probability that a bond exists. It means that the selected state has a high degree of membership in the chemically defined category.

2.3 Chemical descriptors

For the present conceptual proposed model, four descriptors are especially useful: bond distance R , electronegativity difference $\Delta\chi$, an electron-sharing descriptor S , and a localization descriptor L . The numerical definition of S or L can be chosen from quantum-chemical analyses such as bond order, integrated density in a bonding region, localization indices, or related topological measures. The fuzzy framework is therefore compatible with several underlying electronic-structure methods.

3. FUZZY MODEL OF CHEMICAL BONDING

3.1 Bond membership

Let B denote the degree of membership of an internuclear region in the category “bonding region”. A simple model combines distance, electron sharing, and an energetic or bond-order descriptor:

$$\mu_B = w_R f_R + w_S f_S + w_E f_E, \quad w_R + w_S + w_E = 1 \quad (4)$$

A Gaussian distance membership, for example, can be written as:

$$f_R(R) = \exp[-(R - R_0)^2/(2\sigma_R^2)] \quad (5)$$

where R_0 is a characteristic equilibrium distance and σ_R controls the width of the chemically relevant region. The function does not claim that a bond disappears abruptly beyond one arbitrary distance; bonding membership decreases continuously.

3.2 Covalency and polarity as independent dimensions

A central feature of the proposed model is that covalency and polarity are not treated as mutually exclusive categories. A bond may have high covalent membership and high polar membership simultaneously. This is chemically important for O–H and N–H bonds. Then,

$$\mu_C = f(S, \Delta\rho, \text{bond order}) \quad (6)$$

$$\mu_P = 1 - \exp(-k|\Delta\chi|) \quad (7)$$

Equation (7) is an illustrative membership function rather than a universal physical law. The parameter k determines how the chosen electronegativity scale is mapped into polarity membership. Quantitative use would require calibration against experimental or computational data.

3.3 Fuzzy linguistic rules

The numerical membership functions can be combined through transparent linguistic rules, as shown in Table 1.

Table 1. Illustrative fuzzy rules for interpreting chemical bonding.

Rule	Fuzzy statement
R1	IF electron sharing is high AND electronegativity difference is low, THEN covalent membership is high.
R2	IF electron sharing is high AND

	electronegativity difference is high, THEN covalent membership is high AND polarity membership is high.
R3	IF localization near one nucleus is high AND electron sharing is low, THEN ionic-character membership is high.
R4	IF electron density between the nuclei is high AND distance is near the equilibrium region, THEN bond membership is high.
R5	IF a nonbonding electron domain is highly localized outside the internuclear region, THEN lone-pair membership is high.

3.4. H₂: The symmetric limit

H₂ is the most direct molecular system for examining the relationship between electron sharing and chemical bonding. The two nuclei are identical, and the ground-state molecule has a $\sigma(1s)$ bonding molecular orbital occupied by two electrons. The molecular electron density is symmetric with respect to exchange of the two nuclei.

Within the fuzzy framework, H₂ is characterized by high electron-sharing membership and very low polarity membership. The important point is that “nonpolar” does not imply “electronically featureless”. The electron density in the internuclear region is precisely what supports the familiar covalent interpretation. Hence:

$$\Psi_{\text{MO}} \approx c_A 1s_A + c_B 1s_B, \quad |c_A| \approx |c_B| \quad (8)$$

$$\mu_C(\text{H}_2) \rightarrow \text{high}; \quad \mu_P(\text{H}_2) \rightarrow \text{low}; \quad \mu_B(\text{H}_2) \rightarrow \text{high} \quad (9)$$

As the H–H distance increases, orbital overlap and stabilization decrease. Rather than defining a single arbitrary distance at which the bond changes from “present” to “absent”, the fuzzy membership can decrease smoothly along the dissociation coordinate.

3.5. H₂O: Polar Covalent Bonding and Molecular Geometry

Water molecule introduces a richer electronic situation. Oxygen is more electronegative than hydrogen, so the O–H bonds exhibit substantial polarity. At the same time, the bonds remain strongly covalent: electronic density is redistributed through molecular orbitals rather than being described adequately as complete electron transfer.

A fuzzy representation can therefore assign simultaneously high membership to the categories “covalent bond” and “polar bond”. This avoids the conceptual trap in which covalent and ionic descriptions are treated as opposite boxes. Bond character is better represented as a continuum.

Water molecule also shows why geometry should be part of a fuzzy molecular description. Its bent structure is coupled to the spatial organization of occupied molecular orbitals and electron density around oxygen. The two O–H bonds are not independent sticks placed at an arbitrary angle; their orientation is connected to the distribution of bonding and nonbonding electron density:

$$\Delta\chi_{\text{OH}} = \chi_{\text{O}} - \chi_{\text{H}} > 0 \quad (10)$$

$$\mu_{\text{angle}} = f(\theta; \theta_0, \sigma\theta) \quad (11)$$

Here θ_0 is a reference angle for the molecular state being described, while $\sigma\theta$ controls the width of the angular membership. In a calibrated model, both parameters could be linked to experimental structures or high-level calculations.

3.6. NH_3 : Three polar bonds and a localized lone pair

Ammonia extends the framework from two bonds to three and introduces a localized lone pair on nitrogen. The molecule is approximately trigonal pyramidal, and the N–H bonds are polar because nitrogen and hydrogen differ in electronegativity.

The lone pair is particularly interesting from the fuzzy perspective. It is not a bond, yet it is an organized region of electron density that influences molecular geometry and reactivity. A localization membership can represent the degree to which an electron domain is concentrated around nitrogen.

The three N–H bonds can also be treated as a coupled set rather than as three completely independent objects. A collective descriptor can represent their similarity and therefore their approximate equivalence in the equilibrium structure. As consequence:

$$\Delta\chi_{\text{NH}} = \chi_{\text{N}} - \chi_{\text{H}} > 0 \quad (12)$$

$$\mu_{\text{LP}} = f(\text{localization, population, spatial confinement}) \quad (13)$$

$$\mu_{\text{sym}} = 1 - \text{Var}(\mu_{\text{B1}}, \mu_{\text{B2}}, \mu_{\text{B3}})/V_{\text{max}} \quad (14)$$

3.7. Comparative Fuzzy Description

Table 2 contains qualitative, normalized descriptors rather than experimental measurements. It illustrates how a fuzzy model organizes molecular information. In an empirical implementation, the membership functions would be calibrated from a defined computational dataset.

Table 2. Qualitative fuzzy characterization of H_2 , H_2O and NH_3 .

Molecule	Bond	Covalent μ	Polarity μ	Localization	Nonbonding domains	Geometry
H ₂	H–H	High	Very low	Low–moderate	None	Linear
H ₂ O	O–H	High	High	Moderate–high near O	Two lone pairs	Bent
NH ₃	N–H	High	Moderate–high	Moderate–high near N	One lone pair	Trigonal pyramidal

Table 2 highlights the principal advantage of the proposed approach: one molecular state can possess substantial membership in several chemically meaningful categories at once. H₂ is dominated by symmetric electron sharing. H₂O combines strong covalent membership with strong polarity and localized nonbonding domains. NH₃ combines polar covalent bonds with a localized lone pair and a pyramidal geometry.

3.8. Computational Implementation

A computational study could begin by optimizing the molecular geometries of H₂, H₂O, and NH₃ with a specified electronic-structure method. Electron density and, where appropriate, an electron-localization descriptor can then be calculated. Bond distances, bond angles, dipole moments, bond orders, and selected integrated density descriptors form a molecular feature vector can also be provided.

Each descriptor is normalized or transformed through an explicitly defined membership function. A fuzzy inference system then maps the descriptor vector onto linguistic chemical properties. A Mamdani system is attractive when interpretability is the main objective, whereas a Sugeno-type system can be convenient for numerical modeling:

$$x = [R, \theta, \Delta\chi, BO, \rho_b, L, \mu_{\text{dipole}}, \dots] \quad (15)$$

$$F(x) = [\mu_B, \mu_C, \mu_P, \mu_I, \mu_{LP}, \mu_{\text{sym}}, \dots] \quad (16)$$

For a normalized electron-sharing descriptor S , a sigmoid membership function for high covalent character can be written as:

$$\mu_C(S) = 1/[1 + \exp(-a(S - S_0))] \quad (17)$$

where S_0 marks the transition region and a controls for its sharpness. Small values produce gradual transitions, while large values approximate a threshold. This provides a direct mathematical connection between binary chemical classification and graded chemical description.

4. WHAT DOES A FUZZY BOND MEAN?

The phrase “fuzzy bond” should be interpreted carefully. The proposed model does not claim that a quantum state is physically uncertain about whether a bond exists. Quantum mechanics supplies the electronic state; fuzzy logic supplies a language for classifying and reasoning about continuous descriptors.

This distinction makes the framework compatible with conventional quantum chemistry. A molecular orbital, electron density, or electron localization function can be calculated without fuzzy logic. Fuzzy logic is applied afterward, to interpret the resulting data. It therefore functions as a semantic layer between numerical electronic structure and chemical reasoning.

This interpretation also clarifies why membership values should not automatically be treated as observables. Two researchers may construct different membership functions for “ionic character” while using the same electron density. If the functions are explicitly defined and validated, both models may be useful, but they answer somewhat different interpretive questions.

4.1. Relationship to conventional bonding models

The complementary roles of conventional bonding descriptions and fuzzy logic are shown in Table 3. The fuzzy approach complements rather than replaces established bonding theories. Valence-bond theory emphasizes localized structures and resonance; molecular orbital theory describes bonding through molecular orbitals; density-based methods provide quantitative electronic structure; and electron-density topology gives spatially resolved descriptors. Fuzzy logic can use outputs from any of these approaches and convert them into graded chemical categories.

Table 3. Complementary roles of conventional bonding descriptions and fuzzy logic.

Framework	Primary object	Typical contribution	Role in fuzzy model
Valence-bond theory	Localized bonding structures	Chemical intuition and resonance	Source of linguistic categories
Molecular orbital theory	Molecular orbitals	Electronic delocalization	Source of orbital descriptors
Electron-density analysis	$\rho(r)$ and derived fields	Spatial interpretation	Source of density/localization descriptors
Fuzzy logic	Membership and rules	Graded semantic interpretation	Integrative classification layer

4.2. Limitations and Methodological Cautions

Several limitations must be acknowledged. First of all, membership functions are model choices and require calibration and validation if the framework is intended to produce quantitative predictions. Second, chemical descriptors can be method-dependent. Bond orders, partitioning schemes, and localization measures do not have one universally accepted definition. Third, a fuzzy membership value

does not automatically possess an energetic interpretation. A high covalent membership should not be read as a direct numerical measure of bond strength unless a validated relationship has been established.

A further limitation concerns the reference state. Electron-density redistribution depends on how reference atomic densities are constructed. Consequently, two density-based fuzzy models can yield different numerical memberships while remaining internally consistent. Finally, the model should not be used to imply that quantum mechanics is incomplete because chemical categories are graded. The grading arises mainly from the mapping between continuous physical quantities and human chemical language.

4.3. Implications for chemical education and molecular modeling

The proposed framework has potential educational value because it makes explicit a point that is often left implicit in introductory chemistry: chemical categories are abstractions built from continuous physical behavior. Students commonly encounter statements such as “electrons are shared” or “electrons are transferred” as if these were mutually exclusive mechanisms. A fuzzy representation shows that electron sharing and charge polarization can coexist.

For molecular modeling, the framework could provide an interpretable interface between high-dimensional electronic-structure data and human-readable chemical descriptions. For a dataset containing many molecular geometries, fuzzy descriptors could be used to track how bond character changes along a reaction coordinate, during molecular distortion, or across a chemical series:

$$\mu P(s) = f[\text{density redistribution}, \Delta\chi, \text{geometry}, \text{electronic response}] \quad (18)$$

4.4. Extension to Reaction Coordinates

Although this article focuses on equilibrium state/geometry molecules, the same formalism can be applied along a reaction coordinate q . Bond membership, polarity, localization, and other descriptors then become functions of q . A reaction can then be represented as a trajectory through a multidimensional fuzzy chemical space:

$$\Gamma(q) = [\mu B(q), \mu C(q), \mu P(q), \mu LP(q), \mu I(q)] \quad (19)$$

Such a representation may be useful for mechanisms in which conventional labels such as polar, radical, or ionic change progressively rather than abruptly. The fuzzy description remains an interpretive framework, while the underlying q -dependent quantities are obtained from electronic-structure calculations or experiment.

5. CONCLUSIONS

A fuzzy-logic description of chemical bonding provides a mathematically explicit way to represent the graded character of molecular electronic structure. Applied to H_2 , H_2O , and NH_3 , the framework emphasizes that covalency, polarity, localization and nonbonding character need not be mutually

exclusive categories. H_2 represents the symmetric limiting case, with strong electron-sharing membership and minimal polarity. H_2O combines strong covalent membership with pronounced polarity and localized nonbonding electron domains whereas NH_3 combines polar covalent bonds with a nitrogen-centered lone pair and a pyramidal molecular arrangement.

The main contribution of the proposed representation is not a new quantum-mechanical equation for the bond, but a new way of organizing information produced by quantum chemistry: fuzzy membership functions can translate continuous descriptors into chemical statements without forcing an artificial binary decision. With appropriate calibration, the approach could be extended to larger molecules, reaction coordinates, spectroscopy, materials chemistry, and machine-learning datasets.

The proposed framework should therefore be regarded as a complementary layer of chemical description. Its scientific value will depend on transparent definitions of descriptors, reproducible membership functions, validation against independent data, and a clear separation between calculated physical quantities and the linguistic categories used to interpret them.

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