Journal of Intelligent Decision and Computational Modelling

www.jidcm.reapress.com

J. Intell. Decis. Comput. Model. Vol. 1, No. 3 (2025) 158–171.

Paper Type: Original Article

Molecular Fuzzy Graphs, Hypergraphs, and Superhypergraphs

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Citation:

Received: 17 February 2024 *Revised: 22 April 2024* *Accepted: 17 June 2024*	Fujita, T. (2025). Molecular Fuzzy graphs, hypergraphs, and superhypergraphs. *Journal of intelligent decision and computational modelling, 1*(3), 158-171.

Abstract

Graph theory provides a framework for clearly representing relationships between objects [1, 2]. In the fields of chemistry and biology, graph-based concepts are widely applied. Hypergraphs generalize classical graphs by allowing hyperedges to connect any nonempty subset of vertices [3]. Superhypergraphs extend this concept by iterating the powerset operation, thereby generating nested layers that capture hierarchical and self-referential structures among collections of vertices [4]. A molecular graph models a molecule with atoms as vertices and bonds as edges, representing its structural connectivity. Fuzzy graphs and fuzzy hypergraphs enrich these structures by assigning membership degrees to vertices and (hyper)edges. In this paper, we introduce definitions of molecular fuzzy graphs, hypergraphs, and superhypergraphs, and examine their properties and potential applications.

Keywords: Fuzzy graphs, Fuzzy hypergraphs, fuzzy superhypergraphs, hypergraphs, superhypergraphs

1|Preliminaries

We record basic notions and notation used throughout. Unless stated otherwise, all graphs are finite, undirected (multiple edges are allowed only when explicitly declared).

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1.1|SuperHyperGraphs

Classical hypergraphs enrich ordinary graphs by allowing an edge to join any finite number of vertices; this makes them apt for modeling multiway relations [5, 3, 6, 7]. A *SuperHyperGraph* pushes this idea further by building vertices and edges from iterated powersets of a ground set; this perspective has recently attracted attention in several settings [8, 9, 4, 10]. Applications have appeared in, e.g., molecular modeling, network analysis, and signal processing [11, 12, 13]. Throughout, the *level* parameter n is a fixed nonnegative integer.

Definition 1.1 (Base set)**.** A *base set* (or ground set) is a fixed finite set S from which higher-level objects are formed:

$$S \;=\; \{\, x \mid x \text{ lies in the chosen domain} \,\}.$$

All constructions below ultimately draw their elements from S.

Definition 1.2 (Powerset)**.** [14, 15] For a set X, its powerset is

$$\mathcal{P}(X) \;=\; \{\, A \mid A \subseteq X \,\}.$$

We also use the nonempty powerset $\mathcal{P}^*(X) := \mathcal{P}(X) \setminus \{\varnothing\}$.

Definition 1.3 (Iterated powerset)**.** [16, 17, 18] For $k \in \mathbb{N}_0$ define

$$\mathcal{P}^{\,0}(X) := X, \qquad \mathcal{P}^{\,k+1}(X) := \mathcal{P}\big(\mathcal{P}^{\,k}(X)\big).$$

Similarly, with nonempty levels,

$$\big(\mathcal{P}^*\big)^0(X) := X, \qquad \big(\mathcal{P}^*\big)^{k+1}(X) := \mathcal{P}^*\big((\mathcal{P}^*)^k(X)\big).$$

Definition 1.4 (Hypergraph [19, 3])**.** A *hypergraph* is a pair $H = (V(H), E(H))$ where $V(H) \neq \varnothing$ and $E(H) \subseteq \mathcal{P}^*(V(H))$. In this paper we work with finite $V(H)$ and finite $E(H)$.

Definition 1.5 (n-SuperHyperGraph)**.** [20, 21, 22, 23] Fix a finite base set V_0 and a level $n \in \mathbb{N}_0$. An *n-SuperHyperGraph* is a pair

$$\mathrm{SHG}^{(n)} = (V, E), \qquad V \subseteq \mathcal{P}^{\,n}(V_0), \quad E \subseteq \mathcal{P}^*(V),$$

where elements of V are the *n-supervertices* and each $e \in E$ is a nonempty set of supervertices (an *n-superedge*).

Example 1.6 (Level $n = 0$: Carboxylate COO^- as a three-center interaction)**.** Let the base (atom) set be

$$V_0 = \{\, C,\ O_1,\ O_2,\ H_1, \dots \}.$$

At level $n = 0$ we take supervertices to be atoms, so choose

$$V = \{\, C,\ O_1,\ O_2 \,\} \;\subseteq\; \mathcal{P}^{\,0}(V_0) = V_0.$$

Define the hyperedge family $E \subseteq \mathcal{P}^*(V)$ by

$$E = \big\{\, e_\pi,\ e_{\sigma,1},\ e_{\sigma,2} \,\big\}, \qquad e_\pi = \{C, O_1, O_2\},\ \ e_{\sigma,1} = \{C, O_1\},\ \ e_{\sigma,2} = \{C, O_2\}.$$

Then $\mathrm{SHG}^{(0)} = (V, E)$ is an n-SuperHyperGraph: e_π models the three–center π-system delocalized over C, O_1, O_2, while $e_{\sigma,1}$ and $e_{\sigma,2}$ represent the corresponding σ-interactions. By construction $V \subseteq \mathcal{P}^{\,0}(V_0)$ and $E \subseteq \mathcal{P}^*(V)$.

Example 1.7 (Level $n = 1$: Water trimer $(H_2O)_3$ as a hydrogen–bonded ring of molecules)**.** Let the base set V_0 list the atoms of three water molecules:

$$V_0 = \{\, O_A, H_{A1}, H_{A2},\ O_B, H_{B1}, H_{B2},\ O_C, H_{C1}, H_{C2} \,\}.$$

At level $n = 1$ we take supervertices to be sets of atoms (i.e., whole molecules). Define

$$M_A = \{O_A, H_{A1}, H_{A2}\}, \quad M_B = \{O_B, H_{B1}, H_{B2}\}, \quad M_C = \{O_C, H_{C1}, H_{C2}\},$$

and set

$$V = \{\, M_A, M_B, M_C \,\} \ \subseteq\ \mathcal{P}^1(V_0) = \mathcal{P}(V_0).$$

Model cooperative hydrogen bonding by the nonempty sets of supervertices

$$E = \left\{\, e_{\text{ring}},\ e_{AB},\ e_{BC},\ e_{CA} \,\right\} \ \subseteq\ \mathcal{P}^*(V),$$

where

$$e_{\text{ring}} = \{M_A, M_B, M_C\}, \qquad e_{AB} = \{M_A, M_B\}, \quad e_{BC} = \{M_B, M_C\}, \quad e_{CA} = \{M_C, M_A\}.$$

Thus $\mathrm{SHG}^{(1)} = (V, E)$ is an n-SuperHyperGraph whose supervertices are molecules (level–1 aggregates of atoms) and whose superedges capture multi–molecule hydrogen–bond interactions, including the three–membered cyclic motif e_{ring}. By construction $V \subseteq \mathcal{P}^1(V_0)$ and $E \subseteq \mathcal{P}^*(V)$.

1.2|Fuzzy n-SuperHyperGraphs

A fuzzy set assigns a membership degree in $[0, 1]$ to each element of a universe [24, 25]. Fuzzy graphs and fuzzy hypergraphs endow vertices and (hyper)edges with such degrees [26, 27, 28, 29, 30, 31, 32]. A fuzzy n-SuperHyperGraph is a higher-level network structure assigning membership degrees to supervertices and superedges for modeling complex relations (cf.[33, 21]).

Definition 1.8 (Fuzzy Graph)**.** A fuzzy graph is a pair $G = (\sigma, \mu)$ on a nonempty finite vertex set V, where $\sigma : V \to [0, 1]$ assigns to each $v \in V$ a vertex–membership degree and $\mu : V \times V \to [0, 1]$ is a fuzzy edge relation satisfying, for all $u, v \in V$,

$$\mu(u, v) \ \le\ \min\{\sigma(u), \sigma(v)\}.$$

This generalizes a crisp graph by allowing uncertainty on vertices and edges.

Example 1.9 (Fuzzy Graph on three vertices)**.** Let $V = \{v_1, v_2, v_3\}$ and define the vertex–membership

$$\sigma(v_1) = 0.90, \qquad \sigma(v_2) = 0.70, \qquad \sigma(v_3) = 0.50.$$

Define the fuzzy edge relation $\mu : V \times V \to [0, 1]$ (symmetric) by

$$\mu = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \end{array} \begin{array}{c} \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{pmatrix} 0.90 & 0.60 & 0.45 \\ 0.60 & 0.70 & 0.40 \\ 0.45 & 0.40 & 0.50 \end{pmatrix} \end{array}.$$

Verification of the constraint $\mu(u, v) \le \min\{\sigma(u), \sigma(v)\}$:

$$\mu(v_1, v_2) = 0.60 \le \min\{0.90, 0.70\} = 0.70, \quad \mu(v_1, v_3) = 0.45 \le \min\{0.90, 0.50\} = 0.50,$$

$$\mu(v_2, v_3) = 0.40 \le \min\{0.70, 0.50\} = 0.50,$$

and $\mu(v_i, v_i) = \sigma(v_i)$ for $i = 1, 2, 3$. Hence $G = (\sigma, \mu)$ is a fuzzy graph.

Definition 1.10 (Fuzzy Hypergraph)**.** A fuzzy hypergraph is a quadruple $G = (V, E, \psi, w)$ where V is the vertex set; $E \subseteq \mathcal{P}(V) \setminus \{\emptyset\}$ is the family of hyperedges; $\psi \in [0, 1]^{|E|\times|V|}$ with $\psi_{e,i}$ the degree that $i \in V$ belongs to $e \in E$, subject to

$$\sum_{i \in V} \psi_{e,i} = 1 \quad (\forall e \in E), \qquad \sum_{e \in E} \psi_{e,i} > 0 \quad (\forall i \in V);$$

and $w : E \to \mathbb{R}_{>0}$ assigns a positive weight to each hyperedge.

Example 1.11 (Fuzzy Hypergraph on four vertices)**.** Let $V = \{x_1, x_2, x_3, x_4\}$ and take the hyperedge family

$$E = \{e_1, e_2\}, \qquad e_1 = \{x_1, x_2, x_3\}, \quad e_2 = \{x_2, x_4\}.$$

Define $\psi \in [0,1]^{|E|\times|V|}$ by

$$(\psi_{e_1,x_1}, \psi_{e_1,x_2}, \psi_{e_1,x_3}, \psi_{e_1,x_4}) = (0.4,\ 0.3,\ 0.3,\ 0),$$
$$(\psi_{e_2,x_1}, \psi_{e_2,x_2}, \psi_{e_2,x_3}, \psi_{e_2,x_4}) = (0,\ 0.5,\ 0,\ 0.5).$$

Then for each $e \in E$, $\sum_{i\in V} \psi_{e,i} = 1$: $0.4 + 0.3 + 0.3 = 1$ for e_1 and $0.5 + 0.5 = 1$ for e_2. Moreover, each vertex participates with positive total degree:

$$\sum_{e\in E} \psi_{e,x_1} = 0.4 > 0, \quad \sum_{e\in E} \psi_{e,x_2} = 0.3 + 0.5 = 0.8 > 0, \quad \sum_{e\in E} \psi_{e,x_3} = 0.3 > 0, \quad \sum_{e\in E} \psi_{e,x_4} = 0.5 > 0.$$

Assign positive weights $w : E \to \mathbb{R}_{>0}$, e.g., $w(e_1) = 2.0$ and $w(e_2) = 1.2$. Thus $G = (V, E, \psi, w)$ is a fuzzy hypergraph.

Definition 1.12 (Fuzzy n-SuperHyperGraph)**.** (cf.[34, 35]) Let $\mathrm{SHG}^{(n)} = (V, E)$ be as above with $V \subseteq \mathcal{P}^n(V_0)$ and $E \subseteq \mathcal{P}^*(V)$. A *fuzzy n-SuperHyperGraph* is a quadruple

$$(V, E, \sigma, \mu),$$

where $\sigma : V \to [0,1]$ assigns a membership degree to each supervertex and $\mu : E \to [0,1]$ assigns a membership degree to each superedge, subject to the appurtenance constraint

$$\mu(e) \ \le \ \min_{v\in e} \sigma(v) \qquad \text{for every } e \in E.$$

Example 1.13 (Fuzzy n-SuperHyperGraph at level $n = 1$)**.** Let the base set be $V_0 = \{a, b, c, d\}$. At level $n = 1$, supervertices are nonempty subsets of V_0. Let

$$A = \{a, b\}, \qquad B = \{b, c\}, \qquad V = \{A, B\} \subseteq \mathcal{P}^1(V_0),$$

and take the superedge family $E = \{e_1, e_2\} \subseteq \mathcal{P}^*(V)$ with

$$e_1 = \{A, B\}, \qquad e_2 = \{A\}.$$

Define the supervertex membership $\sigma : V \to [0,1]$ by

$$\sigma(A) = 0.80, \qquad \sigma(B) = 0.60,$$

and the superedge membership $\mu : E \to [0,1]$ by

$$\mu(e_1) = 0.55, \qquad \mu(e_2) = 0.78.$$

Verification of the appurtenance constraint $\mu(e) \le \min_{v\in e} \sigma(v)$:

$$\mu(e_1) = 0.55 \ \le \ \min\{\sigma(A), \sigma(B)\} = \min\{0.80, 0.60\} = 0.60,$$
$$\mu(e_2) = 0.78 \ \le \ \min\{\sigma(A)\} = 0.80.$$

Hence (V, E, σ, μ) is a fuzzy 1-SuperHyperGraph.

1.3|Molecular Graph

A molecular graph models a molecule with atoms as vertices and bonds as edges, representing its structural connectivity [36, 37, 38, 39, 40, 41]. Related concepts include molecular hypergraphs [11, 42, 43, 44], which extend this framework to capture higher-order interactions among multiple atoms simultaneously.

Definition 1.14 (Molecular Graph)**.** [36, 37] A *molecular graph* is a finite, simple, undirected graph $G = (V, E)$ in which each vertex $v \in V$ represents an atom and each edge $e = \{u, v\} \in E$ represents a chemical bond between atoms u and v. (Optionally, vertex/edge labels may encode atom types and bond types or orders.)

Example 1.15 (Molecular Graph example: Methane (CH_4) connectivity)**.** A molecular graph is a finite simple undirected graph whose vertices are atoms and edges are chemical bonds. For methane, let

$$V = \{C, H_1, H_2, H_3, H_4\}, \qquad E = \big\{\{C, H_1\}, \{C, H_2\}, \{C, H_3\}, \{C, H_4\}\big\}.$$

Then $G = (V, E)$ captures the tetrahedral connectivity of CH_4 without imposing any edge orientation.

1.4|Fuzzy Molecular Graph

A fuzzy molecular graph assigns $[0,1]$ membership degrees to atoms and bonds on a molecular graph, modeling uncertainty in structure (cf.[45, 46, 47, 48]).

Definition 1.16 (Fuzzy Molecular Graph)**.** (cf.[45, 46, 47, 48]) Fix finite attribute sets Σ_V (atom attributes such as element, charge, isotope) and Σ_E (bond attributes such as order or type). A *fuzzy molecular graph* is a sextuple

$$\mathcal{M}_F = (V, E, \lambda_V, \lambda_E, \sigma, \mu),$$

where

- V is a finite set of *atoms*;
- $E \subseteq \big\{\{u,v\} : u,v \in V,\ u \neq v\big\}$ is a finite set of *(undirected) bonds*;
- $\lambda_V : V \to \Sigma_V$ assigns an attribute to each atom;
- $\lambda_E : E \to \Sigma_E$ assigns an attribute to each bond;
- $\sigma : V \to [0,1]$ is the *vertex (atom) membership* function;
- $\mu : E \to [0,1]$ is the *edge (bond) membership* function.

These membership functions satisfy the standard fuzzy-graph consistency constraint

$$\mu(\{u,v\}) \ \leq\ \min\{\sigma(u), \sigma(v)\} \qquad \text{for every } \{u,v\} \in E.$$

We call $(V, E, \lambda_V, \lambda_E)$ the *underlying (crisp) molecular graph* of $\mathcal{M}_F$. A crisp molecular graph is recovered as the special case $\sigma \equiv 1$ and $\mu = \mathbf{1}_E$ (the indicator of E).

Incidence-aware variant (optional). One may additionally specify an *incidence membership* $\psi : V \times E \to [0,1]$ with

$$\psi(v,e) = 0 \ \text{ if } v \notin e, \qquad \psi(v,e) \ \leq\ \min\{\,\sigma(v), \mu(e)\,\} \ \text{ for all } (v,e) \in V \times E,$$

to explicitly grade the strength with which atom v participates in bond e.

Example 1.17 (Tautomeric proton shift (keto–enol equilibrium))**.** Consider a three-atom fragment capturing the migrating proton in a keto–enol pair. Let

$$V = \{O_1,\ C_\alpha,\ H^*\}, \qquad E = \big\{\{O_1, H^*\},\ \{C_\alpha, H^*\}\big\}.$$

Choose finite attribute sets $\Sigma_V = \{\mathrm{O}, \mathrm{C}, \mathrm{H}\}$ and $\Sigma_E = \{\text{single}\}$ and define labels

$$\lambda_V(O_1) = \mathrm{O},\ \lambda_V(C_\alpha) = \mathrm{C},\ \lambda_V(H^*) = \mathrm{H}, \qquad \lambda_E(\{O_1, H^*\}) = \lambda_E(\{C_\alpha, H^*\}) = \text{single}.$$

A fuzzy molecular graph $\mathcal{M}_F = (V, E, \lambda_V, \lambda_E, \sigma, \mu)$ modeling the time-averaged population may be specified by

$$\sigma(O_1) = \sigma(C_\alpha) = \sigma(H^*) = 1.00,$$

$$\mu(\{O_1, H^*\}) = 0.70, \qquad \mu(\{C_\alpha, H^*\}) = 0.30.$$

The appurtenance constraint holds since, for each edge $e \in E$,

$$\mu(e) \ \leq\ \min\{\sigma(\text{its endpoints})\} = \min\{1,1\} = 1.$$

Interpretation: the proton spends 70% of the time bound to O_1 (enol-like) and 30% to C_α (keto-like), while all three atoms are always present ($\sigma \equiv 1$).

Example 1.18 (Crystallographic partial occupancy of lattice water)**.** In many crystal structures, a solvent water site is partially occupied. Let a single water molecule at a lattice site be modeled by

$$V = \{O_w,\ H_{w1},\ H_{w2}\}, \qquad E = \big\{\{O_w, H_{w1}\},\ \{O_w, H_{w2}\}\big\}.$$

With $\Sigma_V = \{\mathrm{O}, \mathrm{H}\}$ and $\Sigma_E = \{\text{single}\}$, set

$$\lambda_V(O_w) = \mathrm{O},\ \lambda_V(H_{wi}) = \mathrm{H}\ (i = 1,2), \qquad \lambda_E(\{O_w, H_{wi}\}) = \text{single}\ (i = 1,2).$$

Suppose the refined site occupancy is 0.35. A consistent fuzzy specification is

$$\sigma(O_w) = \sigma(H_{w1}) = \sigma(H_{w2}) = 0.35, \qquad \mu(\{O_w, H_{w1}\}) = 0.30, \quad \mu(\{O_w, H_{w2}\}) = 0.28,$$

which satisfies, for each bond,

$$\mu(\{O_w, H_{wi}\}) \ \le \ \min\{\sigma(O_w), \sigma(H_{wi})\} = \min\{0.35, 0.35\} = 0.35 \ \ (i = 1, 2).$$

Interpretation: the water molecule occupies the site 35% of the time; when present, the O–H bonds are realized with degrees consistent with that partial occupancy.

2|Main Results

As the main outcome of this paper, we introduce definitions of new graph classes and examine their properties.

2.1|Fuzzy Molecular HyperGraph

A fuzzy molecular hypergraph represents atoms and hyperbonds with graded memberships, extending molecular graphs to uncertain multi-center chemical interactions.

Definition 2.1 (Fuzzy Molecular HyperGraph (FMHG))**.** Fix finite attribute sets Σ_V (atom attributes) and Σ_E (hyperbond attributes). A *fuzzy molecular hypergraph* is a septuple

$$\mathcal{M}_{FH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi),$$

where

- V is a finite set of atoms;
- $E \subseteq \mathcal{P}(V) \setminus \{\varnothing\}$ is a finite family of (undirected) *hyperbonds*;
- $\lambda_V : V \to \Sigma_V$ and $\lambda_E : E \to \Sigma_E$ assign chemical attributes to atoms and hyperbonds;
- $\sigma : V \to [0, 1]$ is the atom membership function;
- $\mu : E \to [0, 1]$ is the hyperbond membership function;
- $\psi : V \times E \to [0, 1]$ is the incidence membership, with $\psi(v, e) = 0$ whenever $v \notin e$,

and the *fuzzy consistency constraints* hold for every $e \in E$:

$$\mu(e) \ \le \ \min_{v \in e} \sigma(v), \qquad \psi(v, e) \ \le \ \min\{\sigma(v), \mu(e)\} \ \text{ for all } v \in e. \tag{1}$$

Remark 2.2. Chemically, $\sigma(v)$ grades the presence/uncertainty of atom v (e.g., partial occupancy), $\mu(e)$ grades the existence/strength of the multi-center interaction e, and $\psi(v, e)$ grades how strongly atom v participates in that interaction.

Example 2.3 (Diborane B_2H_6: three-center two-electron (3c–2e) B–H–B bridges)**.** (cf.[49, 50]) Let

$$V = \{B_1, B_2, H_{t1}, H_{t2}, H_{t3}, H_{t4}, H_{b1}, H_{b2}\},$$

where $H_{t\bullet}$ are terminal hydrogens and $H_{b\bullet}$ are bridging hydrogens. Take

$$E = \{e_{b1}, e_{b2}, e_{t1}, e_{t2}, e_{t3}, e_{t4}\} \subseteq \mathcal{P}(V) \setminus \{\varnothing\},$$

with

$$e_{b1} = \{B_1, H_{b1}, B_2\}, \quad e_{b2} = \{B_1, H_{b2}, B_2\}, \qquad e_{ti} = \{B_{\alpha(i)}, H_{ti}\} \ (i = 1, \ldots, 4),$$

where $\alpha(1) = \alpha(2) = 1$ and $\alpha(3) = \alpha(4) = 2$. Choose finite attribute sets $\Sigma_V = \{\mathrm{B}, \mathrm{H}\}$ and $\Sigma_E = \{\text{3c–2e}, \text{2c–2e}\}$ and define labels by element/bond type: $\lambda_V(B_j) = \mathrm{B}$, $\lambda_V(H_\bullet) = \mathrm{H}$, $\lambda_E(e_{b\bullet}) = \text{3c–2e}$, $\lambda_E(e_{t\bullet}) = \text{2c–2e}$. Let atom membership and hyperbond membership be

$$\sigma(B_1) = \sigma(B_2) = 1, \quad \sigma(H_{ti}) = 1 \ (i = 1, \ldots, 4), \quad \sigma(H_{b1}) = \sigma(H_{b2}) = 0.90,$$

$$\mu(e_{b1}) = 0.80, \quad \mu(e_{b2}) = 0.75, \qquad \mu(e_{ti}) = \begin{cases} 0.95, & i = 1, 2, \\ 0.92, & i = 3, 4. \end{cases}$$

Define the incidence membership ψ on vertices contained in each hyperedge by

$$\psi(v, e) = \mu(e) \quad \text{if } v \in e, \qquad \psi(v, e) = 0 \quad \text{if } v \notin e.$$

Verification of constraints for a representative edge: for $e_{b1} = \{B_1, H_{b1}, B_2\}$,

$$\min_{v \in e_{b1}} \sigma(v) = \min\{1, 0.90, 1\} = 0.90, \quad \mu(e_{b1}) = 0.80 \leq 0.90, \quad \psi(v, e_{b1}) = 0.80 \leq \min\{\sigma(v), \mu(e_{b1})\} \ (v \in e_{b1}).$$

All other edges satisfy the same inequalities by construction. Hence $\mathcal{M}_{FH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi)$ is an FMHG for diborane.

Example 2.4 (μ_3-Oxo trinuclear iron core Fe_3O)**.** (cf.[51]) Let $V = \{\mathrm{Fe}_1, \mathrm{Fe}_2, \mathrm{Fe}_3, O_{\mu_3}\}$ and

$$E = \{e_{\mu_3},\ e_1, e_2, e_3\}, \quad e_{\mu_3} = \{\mathrm{Fe}_1, \mathrm{Fe}_2, \mathrm{Fe}_3, O_{\mu_3}\}, \quad e_i = \{\mathrm{Fe}_i, O_{\mu_3}\} \ (i = 1, 2, 3).$$

Let $\Sigma_V = \{\mathrm{Fe}, \mathrm{O}\}$ and $\Sigma_E = \{\mu_3\text{-oxo}, \mathrm{Fe–O}\}$ with labels $\lambda_V(\mathrm{Fe}_i) = \mathrm{Fe}$, $\lambda_V(O_{\mu_3}) = \mathrm{O}$, $\lambda_E(e_{\mu_3}) = \mu_3$-oxo, $\lambda_E(e_i) = \mathrm{Fe–O}$. Choose

$$\sigma(\mathrm{Fe}_i) = 1 \ (i = 1, 2, 3), \qquad \sigma(O_{\mu_3}) = 1,$$

$$\mu(e_{\mu_3}) = 0.85, \qquad \mu(e_1) = 0.90,\ \mu(e_2) = 0.88,\ \mu(e_3) = 0.89,$$

and set $\psi(v, e) = \mu(e)$ if $v \in e$ and 0 otherwise. Then for e_{μ_3},

$$\min_{v \in e_{\mu_3}} \sigma(v) = 1 \ \Rightarrow\ \mu(e_{\mu_3}) = 0.85 \leq 1, \quad \psi(v, e_{\mu_3}) = 0.85 \leq \min\{1, 0.85\} = 0.85 \ (v \in e_{\mu_3}),$$

and similarly for each pairwise Fe–O edge e_i. Thus this FMHG represents the multi-center μ_3-oxo interaction consistently.

Example 2.5 (Benzene C_6H_6: delocalized π-sextet)**.** (cf.[52]) Let $V = \{C_1, \ldots, C_6, H_1, \ldots, H_6\}$ and consider the hyperedge family

$$E = \{e_\pi,\ e_{\sigma,1}, \ldots, e_{\sigma,6}\},$$

where the delocalized π-system is modeled by

$$e_\pi = \{C_1, C_2, C_3, C_4, C_5, C_6\},$$

and each σ C–H bond by $e_{\sigma,i} = \{C_i, H_i\}$, $i = 1, \ldots, 6$. Let $\Sigma_V = \{\mathrm{C}, \mathrm{H}\}$ and $\Sigma_E = \{\pi\text{-system}, \mathrm{C–H}\}$ with obvious labels. Choose full atom presence

$$\sigma(C_i) = \sigma(H_i) = 1 \qquad (i = 1, \ldots, 6),$$

and hyperbond memberships

$$\mu(e_\pi) = 0.90, \qquad \mu(e_{\sigma,i}) = 0.98 \ \ (i = 1, \ldots, 6).$$

Define $\psi(v, e) = \mu(e)$ if $v \in e$ and 0 otherwise. Then

$$\min_{v \in e_\pi} \sigma(v) = 1 \ \Rightarrow\ \mu(e_\pi) = 0.90 \leq 1, \qquad \psi(v, e_\pi) = 0.90 \leq \min\{1, 0.90\} = 0.90 \ (v \in e_\pi),$$

and for each $e_{\sigma,i}$,

$$\min_{v \in e_{\sigma,i}} \sigma(v) = 1 \ \Rightarrow\ \mu(e_{\sigma,i}) = 0.98 \leq 1, \quad \psi(v, e_{\sigma,i}) = 0.98 \leq \min\{1, 0.98\} = 0.98.$$

Hence $(V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi)$ is an FMHG encoding the six-center π-delocalization together with the local C–H interactions.

Theorem 2.6 (FMHG generalizes the fuzzy molecular graph)**.** *There exist maps*

$$I : \{\textit{fuzzy molecular graphs}\} \longrightarrow \{\textit{FMHGs}\}, \qquad U : \{\textit{FMHGs}\} \longrightarrow \{\textit{fuzzy molecular graphs}\},$$

such that for every fuzzy molecular graph $\mathcal{M}_F$ we have $U\big(I(\mathcal{M}_F)\big) = \mathcal{M}_F$. Hence fuzzy molecular graphs embed as a special case of FMHGs (hyperedges of size 2), so FMHGs strictly generalize fuzzy molecular graphs.

Proof: Let $\mathcal{M}_F = (V, E^{(2)}, \lambda_V, \lambda_E^{(2)}, \sigma, \mu^{(2)})$ be a fuzzy molecular graph. Define

$$I(\mathcal{M}_F) \;:=\; \big(V,\ E := E^{(2)},\ \lambda_V,\ \lambda_E := \lambda_E^{(2)},\ \sigma,\ \mu := \mu^{(2)},\ \psi\big),$$

where for all $e = \{u, v\} \in E = E^{(2)}$ we put

$$\psi(u, e) \;:=\; \mu^{(2)}(e), \qquad \psi(v, e) \;:=\; \mu^{(2)}(e), \qquad \psi(x, e) := 0 \;\; (x \in V \setminus e).$$

We verify the FMHG constraints (1). Since $\mu^{(2)}(e) \le \min\{\sigma(u), \sigma(v)\}$ by the fuzzy molecular graph condition, we get

$$\mu(e) = \mu^{(2)}(e) \;\le\; \min_{x \in e} \sigma(x),$$

and for $x \in e$,

$$\psi(x, e) = \mu^{(2)}(e) \;\le\; \min\{\sigma(x), \mu^{(2)}(e)\} \;=\; \min\{\sigma(x), \mu(e)\}.$$

Also $\psi(x, e) = 0$ when $x \notin e$ by definition. Thus $I(\mathcal{M}_F)$ is an FMHG.

Conversely, for an FMHG $\mathcal{M}_{FH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi)$ define

$$U(\mathcal{M}_{FH}) \;:=\; \big(V,\ E^{(2)},\ \lambda_V,\ \lambda_E^{(2)},\ \sigma,\ \mu^{(2)}\big),$$

where $E^{(2)} := \{\, e \in E :\ |e| = 2 \,\}$, $\lambda_E^{(2)} := \lambda_E|_{E^{(2)}}$, and $\mu^{(2)} := \mu|_{E^{(2)}}$. For any $e = \{u, v\} \in E^{(2)}$, the FMHG axiom gives $\mu^{(2)}(e) = \mu(e) \le \min\{\sigma(u), \sigma(v)\}$, so $U(\mathcal{M}_{FH})$ is a fuzzy molecular graph.

Finally, applying U to $I(\mathcal{M}_F)$ does not change V, $E^{(2)}$, λ_V, $\lambda_E^{(2)}$, σ, or $\mu^{(2)}$ because $I(\mathcal{M}_F)$ uses only size-2 hyperedges with the same labels and memberships. Hence $U\big(I(\mathcal{M}_F)\big) = \mathcal{M}_F$. □

Theorem 2.7 (FMHG is a fuzzy hypergraph)**.** *For any fuzzy molecular hypergraph $\mathcal{M}_{FH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi)$, the quintuple*

$$\mathcal{H} := \big(V, E, \sigma, \mu, \psi\big)$$

is a fuzzy hypergraph.

Proof: By definition of FMHG, $E \subseteq \mathcal{P}(V) \setminus \{\varnothing\}$, $\sigma : V \to [0, 1]$, $\mu : E \to [0, 1]$, and $\psi : V \times E \to [0, 1]$ with $\psi(v, e) = 0$ for $v \notin e$. It remains to verify the fuzzy constraints.

Fix $e \in E$ and enumerate $e = \{v_1, \ldots, v_k\}$, $k \ge 1$. Put $\alpha_i := \sigma(v_i) \in [0, 1]$ and $\beta := \mu(e) \in [0, 1]$. The FMHG axiom yields

$$\beta = \mu(e) \;\le\; \min_{1 \le i \le k} \alpha_i,$$

which is exactly the hyperedge–vertex compatibility for fuzzy hypergraphs. For each $j \in \{1, \ldots, k\}$, the incidence constraint in FMHG gives

$$\psi(v_j, e) \;\le\; \min\{\sigma(v_j), \mu(e)\} \;=\; \min\{\alpha_j, \beta\} \;\in [0, 1].$$

Thus all fuzzy hypergraph axioms hold, and $\mathcal{H}$ is a fuzzy hypergraph. □

Proposition 2.8 (Crisp recovery and conservative extension)**.** *If $\sigma \equiv 1$, $\mu(e) \in \{0, 1\}$ and $\psi(v, e) = \mathbf{1}_{\{v \in e\}} \cdot \mu(e)$, then $\mathcal{M}_{FH}$ reduces to a (crisp) labeled molecular hypergraph $(V, E, \lambda_V, \lambda_E)$. If, in addition, all hyperedges have size 2, one recovers a (crisp) labeled molecular graph.*

Proof: With $\sigma \equiv 1$ and $\mu(e) \in \{0, 1\}$, the inequality $\mu(e) \le \min_{v \in e} \sigma(v)$ is automatic. The chosen ψ satisfies $\psi(v, e) = 0$ for $v \notin e$ and $\psi(v, e) = 1$ for $v \in e$ when $\mu(e) = 1$, hence $\psi(v, e) \le \min\{\sigma(v), \mu(e)\}$ holds with equality when $v \in e$ and $\mu(e) = 1$. Therefore (V, E) is a crisp hypergraph carrying labels λ_V, λ_E. If $|e| = 2$ for all e, this is precisely a (crisp) labeled molecular graph. □

2.2|Fuzzy Molecular SuperHyperGraph

A fuzzy molecular superhypergraph assigns membership degrees in $[0,1]$ to supervertices (atoms, groups, or higher aggregates) and to superedges (multi–center interactions) at a fixed hierarchical level, thereby extending fuzzy molecular hypergraphs in a type–consistent way.

Definition 2.9 (Fuzzy Molecular SuperHyperGraph (level n))**.** Fix $n \in \mathbb{N}_0$, a finite base (atom) set V_0, and finite attribute sets Σ_V (vertex/aggregate attributes) and Σ_E (edge/interaction attributes). A *fuzzy molecular superhypergraph at level* n is an octuple

$$\mathcal{M}_{FSH}^{(n)} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi; V_0)$$

consisting of:

- a finite level–n vertex set $V \subseteq \mathcal{P}^n(V_0)$ (the n–*supervertices*);
- a finite edge family $E \subseteq \mathcal{P}^*(V)$ (each $e \in E$ is a nonempty set of supervertices);
- label maps $\lambda_V : V \to \Sigma_V$ and $\lambda_E : E \to \Sigma_E$;
- membership maps $\sigma : V \to [0,1]$ (vertex membership) and $\mu : E \to [0,1]$ (edge membership);
- an incidence membership $\psi : V \times E \to [0,1]$ with $\psi(v,e) = 0$ whenever $v \notin e$;

subject to the fuzzy consistency constraints, for every $e \in E$ and $v \in V$,

$$\mu(e) \;\le\; \min_{u \in e} \sigma(u), \qquad \psi(v,e) \;\le\; \min\{\sigma(v), \mu(e)\} \;\text{ if } v \in e. \tag{2}$$

Remark 2.10. Chemically, $n = 0$ models individual atoms; $n = 1$ may group atoms into functional moieties; larger n support hierarchical assemblies. The functions σ, μ, and ψ quantify presence/strength and participation under uncertainty.

Example 2.11 (Level $n = 1$: Serine–histidine–aspartate catalytic triad in a serine protease)**.** (cf.[53]) Let the base atom set V_0 collect all atoms of three residues Ser_{195}, His_{57}, and Asp_{102}. At level $n = 1$, supervertices are nonempty subsets of V_0; take the residue–level aggregates

$$S = \{\text{atoms of } \mathrm{Ser}_{195}\}, \quad H = \{\text{atoms of } \mathrm{His}_{57}\}, \quad D = \{\text{atoms of } \mathrm{Asp}_{102}\},$$

and set $V = \{S, H, D\} \subseteq \mathcal{P}^1(V_0)$. Let the superedge family be

$$E = \{\, e_{\text{triad}},\ e_{SH},\ e_{HD} \,\} \subseteq \mathcal{P}^*(V), \qquad e_{\text{triad}} = \{S, H, D\},\ \ e_{SH} = \{S, H\},\ \ e_{HD} = \{H, D\}.$$

Choose label sets $\Sigma_V = \{\text{Ser}, \text{His}, \text{Asp}\}$ and $\Sigma_E = \{\text{charge relay}, \text{H-bond}\}$ and define

$$\lambda_V(S) = \text{Ser},\ \lambda_V(H) = \text{His},\ \lambda_V(D) = \text{Asp}, \quad \lambda_E(e_{\text{triad}}) = \text{charge relay},\ \lambda_E(e_{SH}) = \lambda_E(e_{HD}) = \text{H-bond}.$$

Pick memberships (steady-state ensemble averages)

$$\sigma(S) = \sigma(H) = \sigma(D) = 1.00, \qquad \mu(e_{\text{triad}}) = 0.85,\ \ \mu(e_{SH}) = 0.90,\ \ \mu(e_{HD}) = 0.88,$$

and define incidence $\psi(v,e) = \mu(e)$ if $v \in e$ and 0 otherwise. Then the FMSHG constraints hold, e.g.

$$\mu(e_{\text{triad}}) = 0.85 \le \min\{1,1,1\} = 1, \qquad \psi(S, e_{\text{triad}}) = 0.85 \le \min\{1, 0.85\} = 0.85,$$

and similarly for H, D and for e_{SH}, e_{HD}. Thus $\mathcal{M}_{FSH}^{(1)} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi; V_0)$ models the triad.

Example 2.12 (Level $n = 1$: Aqueous first hydration shell of Na^+)**.** (cf.[54]) Let V_0 contain the ion Na and three water molecules with atoms $W_i = \{O_i, H_{i1}, H_{i2}\}$ for $i = 1, 2, 3$. At level $n = 1$ define the supervertices

$$N = \{\text{Na}\}, \quad M_1 = W_1, \quad M_2 = W_2, \quad M_3 = W_3,$$

and set $V = \{N, M_1, M_2, M_3\} \subseteq \mathcal{P}^1(V_0)$. Use the superedges

$$E = \{\, e_{\text{shell}},\ e_1, e_2, e_3 \,\} \subseteq \mathcal{P}^*(V), \qquad e_{\text{shell}} = \{N, M_1, M_2, M_3\},\ \ e_i = \{N, M_i\}.$$

Take $\Sigma_V = \{\text{ion}, \text{water}\}$ and $\Sigma_E = \{\text{first-shell}, \text{ion–water}\}$ with

$$\lambda_V(N) = \text{ion},\ \lambda_V(M_i) = \text{water}; \qquad \lambda_E(e_{\text{shell}}) = \text{first-shell},\ \lambda_E(e_i) = \text{ion–water}.$$

Choose memberships reflecting partial residence

$$\sigma(N) = 1.00, \quad \sigma(M_1) = 0.95,\ \sigma(M_2) = 0.90,\ \sigma(M_3) = 0.85,$$
$$\mu(e_{\text{shell}}) = 0.80, \qquad \mu(e_1) = 0.88,\ \mu(e_2) = 0.84,\ \mu(e_3) = 0.78,$$

and let $\psi(v, e) = \mu(e)$ if $v \in e$ and 0 otherwise. Check, e.g.,

$$\mu(e_{\text{shell}}) = 0.80 \le \min\{1.00, 0.95, 0.90, 0.85\} = 0.85, \quad \psi(M_3, e_{\text{shell}}) = 0.80 \le \min\{0.85, 0.80\} = 0.80,$$

and for e_3,

$$\mu(e_3) = 0.78 \le \min\{1.00, 0.85\} = 0.85, \quad \psi(N, e_3) = 0.78 \le \min\{1.00, 0.78\} = 0.78.$$

Hence $(V, E, \sigma, \mu, \psi)$ satisfies the FMSHG constraints.

Example 2.13 (Level $n = 2$: SDS micelle with a water corona)**.** (cf.[55]) Let V_0 collect atoms of k sodium dodecyl sulfate (SDS) molecules M_i $(i = 1, \dots, k)$ and m water molecules W_j $(j = 1, \dots, m)$. At level $n = 1$, view each molecule as a supervertex: $\widetilde{M}_i = M_i$, $\widetilde{W}_j = W_j$, so $\widetilde{V} = \{\widetilde{M}_1, \dots, \widetilde{M}_k, \widetilde{W}_1, \dots, \widetilde{W}_m\} \subseteq \mathcal{P}^1(V_0)$. At level $n = 2$, define two aggregate supervertices (sets of level–1 objects)

$$C = \{\widetilde{M}_1, \dots, \widetilde{M}_k\} \quad \text{(surfactant cluster)}, \qquad W = \{\widetilde{W}_1, \dots, \widetilde{W}_m\} \quad \text{(hydration shell)},$$

and take $V = \{C, W\} \subseteq \mathcal{P}^2(V_0)$. Use the superedges

$$E = \{\, e_{\text{micelle}},\ e_{\text{interface}} \,\} \subseteq \mathcal{P}^*(V), \qquad e_{\text{micelle}} = \{C\},\ \ e_{\text{interface}} = \{C, W\}.$$

Let $\Sigma_V = \{\text{cluster}, \text{shell}\}$ and $\Sigma_E = \{\text{aggregate}, \text{contact}\}$ with

$$\lambda_V(C) = \text{cluster},\ \lambda_V(W) = \text{shell}, \qquad \lambda_E(e_{\text{micelle}}) = \text{aggregate},\ \lambda_E(e_{\text{interface}}) = \text{contact}.$$

Choose memberships

$$\sigma(C) = 0.95, \qquad \sigma(W) = 0.90, \qquad \mu(e_{\text{micelle}}) = 0.92, \quad \mu(e_{\text{interface}}) = 0.80,$$

and set $\psi(v, e) = \mu(e)$ if $v \in e$ and 0 otherwise. Then

$$\mu(e_{\text{micelle}}) = 0.92 \le \min\{\sigma(C)\} = 0.95, \quad \mu(e_{\text{interface}}) = 0.80 \le \min\{0.95, 0.90\} = 0.90,$$

and, for incidence,

$$\psi(C, e_{\text{interface}}) = 0.80 \le \min\{0.95, 0.80\} = 0.80, \quad \psi(W, e_{\text{interface}}) = 0.80 \le \min\{0.90, 0.80\} = 0.80.$$

Hence $\mathcal{M}^{(2)}_{FSH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi; V_0)$ is a valid level–2 FMSHG capturing a micelle and its water corona.

Theorem 2.14 (FMSHG generalizes the fuzzy molecular hypergraph)**.** *When $n = 0$ (so $\mathcal{P}^0(V_0) = V_0$), every fuzzy molecular hypergraph $\mathcal{M}_{FH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi)$ with $V \subseteq V_0$ and $E \subseteq \mathcal{P}^*(V)$ embeds into a fuzzy molecular superhypergraph $\mathcal{M}^{(0)}_{FSH}$ such that a suitable forgetful map returns $\mathcal{M}_{FH}$ exactly.*

Proof: Define the embedding

$$I_0(\mathcal{M}_{FH}) := \big(V,\ E,\ \lambda_V,\ \lambda_E,\ \sigma,\ \mu,\ \psi;\ V_0\big),$$

viewing $V \subseteq V_0$ and $E \subseteq \mathcal{P}^*(V) = \mathcal{P}^*(\mathcal{P}^0(V_0))$. The constraints (2) are exactly the fuzzy molecular hypergraph axioms, hence $I_0(\mathcal{M}_{FH})$ is a valid level–0 FMSHG.

Define the forgetful map

$$U_0\big(V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi; V_0\big) := (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi).$$

Then $U_0 \circ I_0 = \text{id}$ on fuzzy molecular hypergraphs, proving that FMSHGs (at $n = 0$) strictly generalize fuzzy molecular hypergraphs. □

Theorem 2.15 (Forgetting labels yields a fuzzy superhypergraph)**.** *Let $\mathcal{M}^{(n)}_{FSH} = (V, E, \lambda_V, \lambda_E, \sigma, \mu, \psi; V_0)$ be a fuzzy molecular superhypergraph at level n. Then the quadruple*

$$\mathsf{FSH}^{(n)} := (V, E, \sigma, \mu)$$

is a fuzzy superhypergraph at level n, i.e.,

$$\mu(e) \ \le\ \min_{v \in e} \sigma(v) \qquad \text{for all } e \in E. \tag{3}$$

Proof: By Definition 2.9, $V \subseteq \mathcal{P}^n(V_0)$ is finite and $E \subseteq \mathcal{P}^*(V)$ is a finite family of nonempty sets of supervertices. The first inequality in (2) is precisely (3), so (V, E, σ, μ) satisfies the fuzzy superhypergraph axiom. □

Proposition 2.16 (Crisp recovery; conservative extension)**.** *If $\sigma \equiv 1$, $\mu(e) \in \{0,1\}$ for all $e \in E$, and $\psi(v,e) = \mathbf{1}_{\{v \in e\}} \cdot \mu(e)$, then $\mathcal{M}_{FSH}^{(n)}$ reduces to a labeled molecular superhypergraph $(V, E, \lambda_V, \lambda_E)$ at level n. For $n = 0$ this is a labeled molecular hypergraph; if, in addition, every $e \in E$ has $|e| = 2$, one recovers a labeled molecular graph. Hence the fuzzy model is a conservative extension of the crisp one.*

Proof: With $\sigma \equiv 1$ and $\mu \in \{0,1\}$, the inequality $\mu(e) \leq \min_{v \in e} \sigma(v) = 1$ is automatic. The chosen ψ is 0 off–incidence and 1 on–incidence when $\mu(e) = 1$, so (2) holds. Forgetting σ, μ, ψ yields the crisp labeled structure. The stated specializations follow immediately. □

3|Conclusion

In this paper, we introduced definitions of molecular fuzzy graphs, hypergraphs, and superhypergraphs, and examined their properties and potential applications. Through these frameworks, it becomes possible to represent hierarchical molecular structures as well as molecular structures with uncertainty.

In future work, we aim to conduct quantitative analyses of the proposed concepts through computational experiments. We also plan to explore possible extensions employing Intuitionistic Fuzzy Graphs [56, 57], Neutrosophic Graphs [58, 59, 60, 61], hyperfuzzy sets [62, 63, 23], and Plithogenic Graphs [64, 65, 66, 67, 68].

Funding

No external funding or financial support was provided for this study.

Acknowledgments

The authors wish to thank all colleagues and mentors whose feedback and encouragement enriched this work. We are grateful to the community of researchers whose foundational contributions informed our developments. Special appreciation goes to the institutions that offered resources and technical infrastructure throughout this project.

Use of Generative AI and AI-Assisted Tools

We use generative AI and AI-assisted tools for tasks such as English grammar checking, and We do not employ them in any way that violates ethical standards.

Data Availability

This manuscript presents purely conceptual work without empirical data. Scholars interested in these ideas are invited to undertake experimental or case-study research to substantiate and extend the proposed frameworks.

Ethical Approval

This paper involves no human or animal subjects and thus did not require ethics committee review or approval.

Conflicts of Interest

The authors declare that there are no competing interests concerning the content or publication of this article.

Disclaimer

The theoretical models and propositions herein have not yet been subjected to practical validation. Readers should independently verify all citations and be aware that inadvertent inaccuracies may remain. The opinions expressed are those of the authors and do not necessarily represent the views of affiliated organizations.

References

[1] Diestel, R. (2025). *Graph theory* (Vol. 173). Springer Nature. https://doi.org/10.1007/978-3-662-70107-2

[2] Gross, J. L., Yellen, J., & Anderson, M. (2018). *Graph theory and its applications*. Chapman and Hall/CRC. https://doi.org/10.1201/9780429425134

[3] Berge, C. (1984). *Hypergraphs: combinatorics of finite sets* (Vol. 45). Elsevier.Hypergraphs, Volume 45 - 1st Edition | Elsevier Shop

[4] Hamidi, M., Smarandache, F., & Davneshvar, E. (2022). Spectrum of superhypergraphs via flows. *Journal of mathematics*, *2022*(1), 9158912. https://doi.org/10.1155/2022/9158912

[5] Akram, M., Gani, A. N., & Saeid, A. B. (2014). Vague hypergraphs. *Journal of intelligent & fuzzy systems*, *26*(2), 647-653. https://doi.org/10.3233/IFS-120756

[6] Feng, Y., You, H., Zhang, Z., Ji, R., & Gao, Y. (2019). Hypergraph neural networks. In *Proceedings of the AAAI conference on artificial intelligence* (Vol. 33, No. 01, pp. 3558-3565). https://doi.org/10.1609/aaai.v33i01.33013558

[7] Gottlob, G., Leone, N., & Scarcello, F. (1999, May). Hypertree decompositions and tractable queries. In *Proceedings of the eighteenth ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems* (pp. 21-32). https://doi.org /10.1145/303976.303979

[8] Valencia, E. M. C., Vásquez, J. P. C., & Lois, F. A. B. (2025). Multineutrosophic analysis of the relationship between survival and business growth in the manufacturing sector of azuay province, 2020–2023, using plithogenic n-superhypergraphs. *Neutrosophic sets and systems*, *84*, 341-355. https://doi.org/10.5281/zenodo.15640723

[9] Ghods, M., Rostami, Z., & Smarandache, F. (2022). Introduction to neutrosophic restricted superhypergraphs and neutrosophic restricted superhypertrees and several of their properties. *Neutrosophic sets and systems*, *50*(1), 28. https://digitalrepository.unm.edu/nss_journal?utm_source=digitalrepository.unm.edu%2Fnss_journa%2Fvol50%2Fiss1%2F28&utm_medium=PDF&utm_campaign=PDFCoverPages

[10] Hamidi, M., Smarandache, F., & Taghinezhad, M. (2023). *Decision making based on valued fuzzy superhypergraphs*. *Computer modeling in engineering & sciences*, *138*(2), 1907-1923. https://doi.org/10.32604/cmes.2023.030284

[11] Fujita, T. (2025). An introduction and reexamination of molecular hypergraph and molecular n-superhypergraph. *Asian journal of physical and chemical sciences*, *13*(3), 1-38. https://doi.org/10.9734/ajopacs/2025/v13i3248

[12] Berrocal Villegas, S. M., Montalvo Fritas, W., Berrocal Villegas, C. R., Flores Fuentes Rivera, M. Y., Espejo Rivera, R., Bautista Puma, L. D., & Macazana Fernández, D. M. (2025). Using plithogenic n-SuperHyperGraphs to assess the degree of relationship between information skills and digital competencies. *Neutrosophic sets and systems*, *84*(1), 41. https://digitalrepository.unm.edu/nss_journal?utm_source=digitalrepository.unm.edu%2Fnss_journal%2Fvol84%2Fiss1%2F41&utm_medium=PDF&utm_campaign=PDFCoverPages

[13] Zhu, S. (2025). Neutrosophic n-superhypernetwork: A new approach for evaluating short video communication effectiveness in media convergence. *Neutrosophic sets and systems*, *85*, 1004-1017. https://fs.unm.edu/nss8/index.php/111/article/download/6351/2689

[14] Al-Odhari, A. (2025). Neutrosophic power-set and neutrosophic hyper-structure of neutrosophic set of three types. *Annals of pure and applied mathematics*, *31*(2), 125-146. http://www.researchmathsci.org/apamart/APAM-v31n2-5.pdf

[15] Hjorth, G. (2005). T. Jech. Set theory. The third millennium edition, revised and expanded. Springer-Verlag, Berlin, 2003, viii+ 769 pp. Bulletin of symbolic logic, 11(2), 243-245. https://doi.org/10.1017/S1079898600003358

[16] Smarandache, F. (2024). The cardinal of the m-powerset of a set of n elements used in the superhyperstructures and neutrosophic superhyperstructures. Systems assessment and engineering management, 2, 19–22. https://doi.org/10.61356/J.SAEM.2024.2436

[17] Das, A. K., Das, R., Das, S., Debnath, B. K., Granados, C., Shil, B., & Das, R. (2025). A comprehensive study of neutrosophic superhyper bci-semigroups and their algebraic significance. Transactions on fuzzy sets and systems, 8(2), 80. https://doi.org/10.71602/tfss.2025.1198050

[18] Smarandache, F. S. (2023). Neutrosophic superhyperstructure: current understanding and future directions, Neutrosophic systems with applications, 12, 68-76. https://doi.org/10.61356/j.nswa.2023.115

[19] Bretto, A. (2013). Hypergraph theory. In An introduction. Mathematical engineering. Cham: Springer, 1, 209-216. https://doi.org/10.1007/978-3-319-00080-0

[20] Huang, M., & Li, F. (2025). Modeling cross-cultural competence in vocational education internationalization using neutrosophic superhyperfunctions and big data driven cultural clusters. Neutrosophic sets and systems, 88(1), 25. https://digitalrepository.unm.edu/nss_journal?utm_source=digitalrepository.unm.edu%2Fnss_journal%2Fvol88%2Fiss1%2F25&utm_medium=PDF&utm_campaign=PDFCoverPages\

[21] Smarandache, F. (2020). *Extension of hypergraph to n-superhypergraph and to plithogenic n-superhypergraph, and extension of hyperalgebra to n-ary (classical-/neutro-/anti-) hyperalgebra*. *Neutrosophic sets and systems, 3*, 291-296. https://B2n.ir/nu4078

[22] Xie, Y. (2025). A neutrosophic superhyper number framework for accurate statistical evaluation of financial performance in high-tech enterprises. *Neutrosophic sets and systems*, *88*(1), 58. https://digitalrepository.unm.edu/nss_journal/vol88/iss1/58?utm_source=digitalrepository.unm.edu%2Fnss_journal%2Fvol88%2Fiss1%2F58&utm_medium=PDF&utm_campaign=PDFCoverPages

[23] Fujita, T., & Smarandache, F. (2024). *Advancing uncertain combinatorics through graphization, hyperization, and uncertainization: Fuzzy, neutrosophic, soft, rough, and beyond: Second volume*. Biblio Publishing. https://doi.org/10.48550/arXiv.2411.17411

[24] Zadeh, L. A. (1965). Fuzzy sets. *Information and control*, *8*(3), 338-353. https://doi.org/10.1016/S0019-9958(65)90241-X

[25] Zadeh, L. A. (1996). Fuzzy logic, neural networks, and soft computing. In *Fuzzy sets, fuzzy logic, and fuzzy systems: selected papers by Lotfi A Zadeh* (pp. 775-782). https://doi.org/10.1142/9789814261302_0040

[26] Nishad, T. M., Al-Hawary, T. A., & Harif, B. M. (2023). General fuzzy graphs. *Ratio mathematica*, *47*, 235-243. http://dx.doi.org/10.23755/rm.v47i0.853

[27] Rosenfeld, A. (1975). Fuzzy graphs. In *Fuzzy sets and their applications to cognitive and decision processes* (pp. 77-95). Academic press. https://doi.org/10.1016/B978-0-12-775260-0.50008-6

[28] Talal, A. H. (2011). Complete fuzzy graphs. *Mathematical combinatorics*, *4*, 26-34. https://fs.unm.edu/IJMC/CompleteFuzzyGraphs.pdf

[29] Farshi, M., & Davvaz, B. (2016). Generalized fuzzy hypergraphs and hypergroupoids. *Filomat*, *30*(9), 2375-2387. https://www.jstor.org/stable/24899255

[30] Samanta, S., & Pal, M. (2012). Bipolar fuzzy hypergraphs. *International journal of fuzzy logic systems*, *2*(1), 17-28. https://doi.org/10.5121/ijfls.2012.2103 17

[31] Akram, M., & Luqman, A. (2020). *Fuzzy hypergraphs and related extensions*. Springer Singapore. https://doi.org/10.1007/978-981-15-2403-5

[32] Mordeson, J. N., & Nair, P. S. (2012). *Fuzzy graphs and fuzzy hypergraphs* (Vol. 46). Physica. https://doi.org/10.1007/978-3-7908-1854-3

[33] Alqahtani, M. (2025). Intuitionistic fuzzy quasi-supergraph integration for social network decision making. *International journal of analysis and applications*, *23*, 137-137. https://doi.org/10.28924/2291-8639-23-2025-137

[34] Fujita, T. (2025). Extensions of multidirected graphs: Fuzzy, neutrosophic, plithogenic, soft, hypergraph, and superhypergraph variants. International journal of topology 2(3), 11. https://doi.org/10.3390/ijt2030011

[35] Fujita, T., & Smarandache, F. (2025). Directed n-superhypergraphs incorporating bipolar fuzzy information: A multi-tier framework for modeling bipolar uncertainty in complex networks. *Neutrosophic sets and systems*, *88*, 164-183. https://doi.org/10.5281/zenodo.15775233

[36] Kearnes, S., McCloskey, K., Berndl, M., Pande, V., & Riley, P. (2016). Molecular graph convolutions: Moving beyond fingerprints. *Journal of computer-aided molecular design*, *30*(8), 595-608. https://doi.org/10.1007/s10822-016-9938-8

[37] Gutman, I., & Estrada, E. (1996). Topological indices based on the line graph of the molecular graph. *Journal of chemical information and computer sciences*, *36*(3), 541-543. https://doi.org/10.1021/ci950143i

[38] You, J., Liu, B., Ying, Z., Pande, V., & Leskovec, J. (2018). Graph convolutional policy network for goal-directed molecular graph generation. In *32nd conference on neural information processing systems (NeurIPS 2018), Montréal, Canada* (pp. 1-12). https://proceedings.neurips.cc/paper_files/paper/2018/file/d60678e8f2ba9c540798ebbde31177e8-Paper.pdf

[39] Gasteiger, J., Groß, J., & Günnemann, S. (2020). Directional message passing for molecular graphs. https://doi.org/10.48550/arXiv.2003.03123 [40] Jin, W., Barzilay, R., & Jaakkola, T. (2020). Hierarchical generation of molecular graphs using structural motifs. In *International conference on machine learning* (pp. 4839-4848). PMLR. https://proceedings.mlr.press/v119/jin20a.html

[41] Jin, W., Barzilay, R., & Jaakkola, T. (2018). Junction tree variational autoencoder for molecular graph generation. In *International conference on machine learning* (pp. 2323-2332). PMLR. https://proceedings.mlr.press/v80/jin18a

[42] Rahman, A., Poirel, C. L., Badger, D. J., & Murali, T. M. (2012, October). Reverse engineering molecular hypergraphs. In *Proceedings of the ACM conference on bioinformatics, computational biology and biomedicine* (pp. 68-75). https://doi.org/10.1145/2382936.2382945

[43] Chen, J., & Schwaller, P. (2024). Molecular hypergraph neural networks. *The journal of chemical physics*, *160*(14). https://doi.org/10.1063/5.0193557

[44] Kajino, H. (2019, May). Molecular hypergraph grammar with its application to molecular optimization. In *international conference on machine learning* (pp. 3183-3191). PMLR. https://proceedings.mlr.press/v97/kajino19a

[45] Lu, J., Zhu, L., & Gao, W. (2022). Cyclic connectivity index of bipolar fuzzy incidence graph. *Open chemistry*, *20*(1), 331-341. https://doi.org/10.1515/chem-2022-0149

[46] Gong, S., & Hua, G. (2021). Topological indices of bipolar fuzzy incidence graph. *Open chemistry*, *19*(1), 894-903. https://doi.org/10.1515/chem-2021-0082/html

[47] Cabrol-Bass, D., Laude, I., Laidboeur, T., & Bangov, I. P. (1995). Fuzzy molecular graphs in a decision support system for molecular structure elucidation. In AIP conference proceedings (Vol. 330, No. 1, pp. 610-617). American Institute of Physics. https://doi.org/10.1063/1.47767

[48] Sebastian, L. (2021). Topological indices of molecular graphs of some anti-cancer drugs. SGS-engineering & sciences, 1(01). https://spast.org/techrep/article/view/604

[49] Lane, C. F. (1976). Reduction of organic compounds with diborane. Chemical reviews, 76(6), 773-799. https://doi.org/doi/pdf/10.1021/cr60304a005

[50] Mulliken, R. S. (1947). The structure of diborane and related molecules. *Chemical reviews*, *41*(2), 207-217. https://doi.org/10.1021/cr60129a002

[51] Lang, J., Hewer, J. M., Meyer, J., Schuchmann, J., van Wüllen, C., & Niedner-Schatteburg, G. (2018). Magnetostructural correlation in isolated trinuclear iron (III) oxo acetate complexes. *Physical chemistry chemical physics*, *20*(24), 16673-16685. https://doi.org/10.1039/C7CP07549A

[52] Allinger, N. L., & Lii, J. H. (1987). Benzene, aromatic rings, van der Waals molecules, and crystals of aromatic molecules in molecular mechanics (MM3). *Journal of computational chemistry*, *8*(8), 1146-1153. https://doi.org/10.1002/jcc.540080812

[53] Rauwerdink, A., & Kazlauskas, R. J. (2015). How the same core catalytic machinery catalyzes 17 different reactions: The serine-histidine-aspartate catalytic triad of α/β-hydrolase fold enzymes. *ACS catalysis*, *5*(10), 6153-6176. https://doi.org/10.1021/acscatal.5b01539

[54] Rempe, S. B., & Pratt, L. R. (2001). The hydration number of Na+ in liquid water. *Fluid phase equilibria*, *183*, 121-132. https://doi.org/10.1016/S0378-3812(01)00426-5

[55] Hammouda, B. (2013). Temperature effect on the nanostructure of SDS micelles in water. *Journal of research of the national institute of standards and technology*, *118*, 151. https://doi.org/10.6028/jres.118.008

[56] Parvathi, R., Karunambigai, M. G., & Atanassov, K. T. (2009). Operations on intuitionistic fuzzy graphs. In *2009 IEEE international conference on fuzzy systems* (pp. 1396-1401). IEEE. https://doi.org/10.1109/FUZZY.2009.5277067

[57] Akram, M., Davvaz, B., & Feng, F. (2013). Intuitionistic fuzzy soft K-algebras. *Mathematics in computer science*, *7*(3), 353-365. https://doi.org/10.1007/s11786-013-0158-5

[58] Akram, M., Malik, H. M., Shahzadi, S., & Smarandache, F. (2018). Neutrosophic soft rough graphs with application. *Axioms*, *7*(1), 14. https://doi.org/10.3390/axioms7010014

[59] Smarandache, F., Broumi, S., Talea, M., & Bakali, A. (2016). Single valued neutrosophic graphs: degree, order and size. In *2016 IEEE international conference on fuzzy systems (FUZZ), pp. 2444-2451.* (p. 2444). IEEE. https://digitalrepository.unm.edu/math_fsp?utm_-source=digitalrepository.unm.edu%2Fmath_fsp%2F404&utm_medium=PDF&utm_campaign=PDFCoverPages

[60] Broumi, S., Talea, M., Bakali, A., & Smarandache, F. (2016). *Interval valued neutrosophic graphs*. Infinite Study. https://fs.unm.edu/IntervalValuedNeutrosophicGraphs-CR12.pdf

[61] Akram, M., & Shahzadi, S. (2017). Neutrosophic soft graphs with application. *Journal of intelligent & fuzzy systems*, *32*(1), 841-858. https://doi.org/10.3233/JIFS-16090

[62] Ghosh, J., & Samanta, T. K. (2012). Hyperfuzzy set and hyperfuzzy group. *International journal of advanced science and technology*, *41*, 27-38. https://www.earticle.net/Article/A206708

[63] Liu, Y. L., Kim, H. S., & Neggers, J. (2017). Hyperfuzzy subsets and subgroupoids. *Journal of intelligent & fuzzy systems*, *33*(3), 1553-1562. https://doi.org/10.3233/JIFS-17104

[64] Sultana, F., Gulistan, M., Ali, M., Yaqoob, N., Khan, M., Rashid, T., & Ahmed, T. (2023). A study of plithogenic graphs: applications in spreading coronavirus disease (covid-19) globally. *Journal of ambient intelligence and humanized computing*, *14*(10), 13139-13159. https://doi.org/10.1007/s12652-022-03772-6

[65] Vizuete, G. X., Gallardo, C. F., & Vizuete, G. (2025). Structured analysis of a generator set lubrication system using vertex articulation in plithogenic n-superhypergraphs. *neutrosophic sets and systems*, *89*(1), 8. https://digitalrepository.unm.edu/nss_journal/vol89/iss1/8/

[66] Crespo-Berti, L. A., Isea Argüelles, J. J., & Villa Zura, M. P. (2025). Effectiveness of dogmatic criminal law reasoning in the permanent structure of the general theory of crime and punishment through plithogenic n-superhypergraphs. *Neutrosophic sets and systems*, *89* (1), 39. https://digitalrepository.unm.edu/nss_journal/vol89/iss1/39/

[67] Takaaki Fujita and Arif Mehmood. (2025). A study on the effectiveness of contradiction values in upside-down logic and de plithogenication within plithogenic sets. *Neutrosophic computing and machine learning, 40*(1), 28–65.

[68] Kandasamy, W. V., Ilanthenral, K., & Smarandache, F. (2020). *Plithogenic Graphs*. Infinite Study. https://fs.unm.edu/Plithogenic-Graphs.pdf