Supplementary Information (S1)

S1. Semi-Quantitative Fuzzy Logic Framework

S1.9. Worked Example of Fuzzy Logic Calculation

This section presents a worked numerical example to demonstrate how fuzzy membership values were derived in a transparent and reproducible manner, without the use of specialized software. The fuzzy logic approach employed here serves as a semi-quantitative framework for ranking the relative importance of catalytic factors rather than a predictive computational model.

S1.9.1. Definition of a Performance Index (PI)

Because catalytic performance in this study is governed by two key outputs—styrene conversion and benzaldehyde selectivity—a simple performance index (PI) was defined to represent overall catalytic effectiveness:

$$PI_i = \frac{1}{2}\left(\frac{Conv_i}{Conv_{max}}\right) + \frac{1}{2}\left(\frac{Sel_i}{Sel_{max}}\right)$$

where:

- $Conv_i$= styrene conversion of catalyst *i* (%),
- Sel_i= benzaldehyde selectivity of catalyst *i* (%),
- $Conv_{max}$= highest conversion observed among all catalysts,
- Sel_{max}= highest benzaldehyde selectivity observed.

From Table 3:

- $Conv_{max} = 49.45\%$ (CSH–Ti),
- $Sel_{max} = 92.81\%$ (CSH–Ag).

Example calculation for CSH–Ti

$$PI_{Ti} = 0.5\left(\frac{49.45}{49.45}\right) + 0.5\left(\frac{60.21}{92.81}\right)$$
$$PI_{Ti} = 0.5(1.00) + 0.5(0.649) = 0.8245$$

The resulting PI values are:

- $PI_{Ti} = 0.8245$
- $PI_{Fe} = 0.5830$
- $PI_{Cu} = 0.5330$
- $PI_{Ag} = 0.6355$

S1.9.2. Example 1: Quantitative Factor — BET Surface Area (F2)

Step A: Normalization of BET Surface Area

To convert BET surface area values into a comparable scale, min–max normalization was applied:

$$S_{i,F2} = \frac{BET_i - BET_{min}}{BET_{max} - BET_{min}}$$

where:

- $BET_{max} = 23.366\ m^2/g$(CSH–Fe),
- $BET_{min} = 3.965\ m^2/g$(CSH–Ag).
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Example for CSH–Ti:

$$S_{Ti,F2} = \frac{21.986 - 3.965}{23.366 - 3.965} = \frac{18.021}{19.401} = 0.929$$

Normalized BET scores:

- $S_{Ti,F2} = 0.929$
- $S_{Fe,F2} = 1.000$
- $S_{Cu,F2} = 0.460$
- $S_{Ag,F2} = 0.000$

Step B: Weighted Influence Score

To assess how strongly BET surface area influences catalytic performance, a weighted average using PI values was calculated:

$$I_{F2} = \frac{\sum_i \quad (S_{i,F2} \cdot PI_i)}{\sum_i \quad PI_i}$$

$$\sum PI_i = 0.8245 + 0.5830 + 0.5330 + 0.6355 = 2.576$$

$$I_{F2} = \frac{(0.929 \cdot 0.8245) + (1.000 \cdot 0.5830) + (0.460 \cdot 0.5330) + (0 \cdot 0.6355)}{2.576}$$

$$I_{F2} = \frac{0.766 + 0.583 + 0.245}{2.576} = 0.619$$

Step C: Mapping to Fuzzy Membership Value

To convert the influence score into a fuzzy membership value while maintaining conservative weighting of physical factors, a linear mapping was applied:

$$\mu_{F2} = 0.30 + 0.70(I_{F2})$$

$$\mu_{F2} = 0.30 + 0.70(0.619) = 0.733$$

This value was rounded to 0.70 (High), consistent with the classification reported in Table 4.

S1.9.3. Example 2: Weak or Non-Linear Factor — Metal Loading (F7)

Metal loading values (wt%) obtained from WDXRF analysis showed no direct linear relationship with catalytic performance. For example:

- CSH–Cu exhibited the highest metal loading but relatively low overall performance,
- CSH–Ti showed the lowest metal loading but the highest performance index.

Although normalized metal loading scores can be calculated similarly to F2, the inverse or inconsistent ranking between metal loading and PI indicates that loading alone is not a dominant factor.

To account for this behavior, a consistency penalty factor (C) was applied:

$$\mu_{F7} = \mu_{raw} \times C$$

where:

- μ_{raw} is the preliminary fuzzy value obtained from normalization,
- C(0–1) reflects the consistency of the factor's trend with catalytic performance.
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Because metal loading showed poor rank consistency with PI, a reduced Cvalue was applied, yielding a final fuzzy membership value of approximately 0.40 (Medium).

This result reflects the chemical reality that metal dispersion and redox accessibility are more important than absolute metal quantity.

S1.9.4. Linguistic Classification

Final fuzzy membership values were categorized using the following linguistic scale:

Linguistic Level	Fuzzy Interval
Low	0.00 – 0.30
Medium	0.31 – 0.69
High	0.70 – 1.00

S1.9.5. Summary

This worked example demonstrates that:

- fuzzy membership values were derived from normalized experimental data,
- weighting was guided by observed catalytic performance,
- no specialized software or predictive modeling was required.

The fuzzy logic framework thus provides a transparent and reproducible method to rank dominant catalytic factors and support structure–activity interpretation.