

Understanding presence of open metal sites in MOFs:

Features Identified by XAI Analysis

- Metals fraction
- Density of solid
- Average Cationic Radius

Metals Fraction:

Explanation: The feature "metals fraction" relate to the proportion of metal ions in the MOF structure that are not fully coordinated, potentially indicating the presence of open metal sites (OMS). A higher fraction of uncoordinated metal ions might suggest a greater number of OMS, which are crucial for adsorption and catalytic applications in MOFs.

Scientific Evidence: The documents discuss the importance of maintaining the structural integrity of MOFs while modifying metal ions to create OMS (Kökçam-Demir et al., 2020). This implies that the fraction of uncoordinated metal ions is a critical factor in the presence of OMS.

Hypothesis: A higher "metals fraction" could correlate with an increased presence of OMS, as it may indicate more metal ions are available to form these sites.

Density of Solid:

Explanation: The "density of solid" feature could influence the presence of OMS by affecting the packing and porosity of the MOF structure. A lower density might suggest a more open framework, potentially allowing for more OMS.

Scientific Evidence: The documents highlight the role of density in differentiating MOF structures and its impact on adsorption

properties (Chung et al., 2019). This suggests that density is a significant factor in the structural characteristics of MOFs, which could relate to the presence of OMS.

Hypothesis: A lower density of solid might be associated with a higher presence of OMS due to increased porosity and structural openness.

Average Cationic Radius:

Explanation: The "average cationic radius" could affect the presence of OMS by influencing the coordination environment and the ability of metal ions to form unsaturated sites. Larger cations might create more space for OMS.

Scientific Evidence: The documents discuss the influence of ionic radius on the binding strength of gases in MOFs, suggesting that cation size affects the coordination environment (Zhou et al., 2008).

Hypothesis: A larger average cationic radius might correlate with a higher presence of OMS, as it could facilitate the formation of unsaturated coordination sites.

Summary

The features identified by the XAI analysis—metals fraction zero, density of solid, and average cationic radius—are potentially related to the presence of open metal sites (OMS) in metal-organic frameworks (MOFs). The "metals fraction zero" feature may indicate the proportion of uncoordinated metal ions, which are directly related to OMS. The "density of solid" could influence the structural openness and porosity of MOFs, affecting the availability of OMS. Lastly, the "average cationic radius" might impact the coordination environment, with larger cations potentially facilitating the formation of OMS. While the documents do not explicitly state these relationships, they provide insights into the structural and chemical factors influencing OMS in MOFs, allowing for the generation of

hypotheses based on the provided information (Kökçam-Demir et al., 2020; Chung et al., 2019; Zhou et al., 2008).

References

1. Kökçam-Demir, U., Goldman, A., Esrafilı, L., Gharib, M., Morsali, A., Weingart, O., & Janiak, C. (2020). Coordinatively unsaturated metal sites (open metal sites) in metal-organic frameworks: design and applications. *Chemical Society Reviews*.
2. Chung, Y. G., Haldoupis, E., Bucior, B. J., Haranczyk, M., Lee, S., Zhang, H., Vogiatzis, K. D., Milisavljevic, M., Ling, S., Camp, J. S., Slater, B., Siepmann, J. I., Sholl, D. S., & Snurr, R. Q. (2019). Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal-Organic Framework Database: CoRE MOF 2019. *Journal of Chemical & Engineering Data*.
3. Zhou, W., Wu, H., & Yildirim, T. (2008). Enhanced H₂ Adsorption in Isostructural Metal-Organic Frameworks with Open Metal Sites: Strong Dependence of the Binding Strength on Metal Ions. *Journal of the American Chemical Society*.

Explanation generated with XpertAI (2024)

Understanding pore limiting diameter in MOFs:

Features Identified by XAI Analysis

- Volume per Atom
- Symmetry Function G1
- Unoccupied Energy Levels Near the Conduction Band Minimum

Volume per Atom:

Explanation: The volume per atom in a material can influence the pore limiting diameter (PLD) in metal-organic frameworks (MOFs) by affecting the overall density and packing of the framework. A larger volume per atom might suggest a more open structure, potentially leading to larger pore sizes, while a smaller volume per atom could indicate tighter packing and smaller pores.

Scientific Evidence: The documents discuss the importance of crystal density as a descriptor for MOF structures, which is related to the volume per atom. Variations in atomic packing, which are influenced by the volume per atom, can lead to different structures and pore sizes (Chung et al., 2019).

Hypothesis: A higher volume per atom in MOFs may correlate with larger pore limiting diameters due to less dense atomic packing, allowing for larger channels within the framework.

Symmetry Function G1:

Explanation: Symmetry functions, such as G1, are often used in computational chemistry to describe the local environment around atoms. While the documents do not explicitly mention Symmetry Function G1, symmetry in general can influence the arrangement of atoms and thus the pore structure in MOFs.

Scientific Evidence: An explicit relationship between Symmetry Function G1 and the pore limiting diameter was not found in the given documents. However, the documents do discuss the geometric properties of MOFs, which are inherently related to symmetry (Haldoupis et al., 2010).

Hypothesis: Symmetry Function G1 may impact the pore limiting diameter by influencing the spatial arrangement of atoms, potentially affecting the uniformity and size of the pores.

Unoccupied Energy Levels Near the Conduction Band Minimum:

Explanation: Unoccupied energy levels near the conduction band minimum can affect the electronic properties of MOFs, which in turn might influence the interaction between the framework and adsorbates. This could indirectly affect the pore limiting diameter by altering the stability and structure of the MOF.

Scientific Evidence: The documents do not explicitly link unoccupied energy levels to the pore limiting diameter. However, they discuss the impact of energy barriers and adsorption properties on MOF performance, which could be related to electronic structure (Haldoupis et al., 2010).

Hypothesis: Unoccupied energy levels near the conduction band minimum may influence the pore limiting diameter by affecting the electronic interactions within the MOF, potentially leading to structural changes that alter pore sizes.

Summary

The relationship between the identified features and the pore limiting diameter in MOFs is complex and not explicitly detailed in the provided documents. The volume per atom is likely to influence the pore limiting diameter through its effect on atomic packing and density, potentially leading to larger or smaller pores depending on the volume. Symmetry Function G1, while not explicitly discussed, could impact the pore structure

by affecting the spatial arrangement of atoms. Unoccupied energy levels near the conduction band minimum might indirectly influence the pore limiting diameter by altering the electronic properties and stability of the MOF. These hypotheses are based on the general principles discussed in the documents, such as the importance of geometric and electronic properties in determining MOF structure and function.

References

1. Chung, Y. G., Haldoupis, E., Bucior, B. J., Haranczyk, M., Lee, S., Zhang, H., Vogiatzis, K. D., Milisavljevic, M., Ling, S., Camp, J. S., Slater, B., Siepmann, J. I., Sholl, D. S., & Snurr, R. Q. (2019). Advances, Updates, and Analytics for the Computation-Ready, Experimental Metal–Organic Framework Database: CoRE MOF 2019.
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Explanation generated with XpertAI (2024)

Understanding toxicity of small molecules:

Features Identified by XAI Analysis

- Presence of a heteroatom bonded to three oxygen atoms
- Presence of a tertiary amine
- Presence of a carbon-oxygen single bond

Presence of a heteroatom bonded to three oxygen atoms:

Explanation: The presence of a heteroatom bonded to three oxygen atoms, such as in a phosphate group, is often associated with significant chemical reactivity due to the electronegative nature of oxygen atoms. This can influence the molecular structure and reactivity, potentially affecting the toxicity of small molecules.

Scientific Evidence: The document discusses the role of oxygen lone pairs in chemical reactivity, particularly in anomeric systems where oxygen atoms interact with strong sigma-acceptors (Alabugin et al., 2021). This suggests that the presence of multiple oxygen atoms bonded to a heteroatom can lead to increased reactivity and potentially influence toxicity.

Hypothesis: The presence of a heteroatom bonded to three oxygen atoms may increase the reactivity of a molecule, thereby influencing its toxicity profile due to potential interactions with biological targets.

Presence of a tertiary amine:

Explanation: Tertiary amines are known for their nucleophilic properties, which can lead to interactions with electrophilic

sites in biological systems. This can result in various biological effects, including potential toxicity.

Scientific Evidence: The SHAP analysis indicates a positive correlation between the presence of a tertiary amine and its impact on the model, suggesting its relevance in toxicity predictions (XpertAI, 2023).

Hypothesis: Tertiary amines may contribute to the toxicity of small molecules through their nucleophilic interactions with biological macromolecules, potentially leading to adverse effects.

Presence of a carbon-oxygen single bond:

Explanation: Carbon-oxygen single bonds are common in various functional groups such as alcohols and ethers. These bonds can influence the solubility, reactivity, and overall chemical behavior of a molecule, which in turn can affect its toxicity.

Scientific Evidence: The SHAP analysis shows a positive correlation between the presence of a carbon-oxygen single bond and its impact on the model, indicating its significance in toxicity predictions (XpertAI, 2023).

Hypothesis: The presence of carbon-oxygen single bonds may affect the toxicity of small molecules by altering their chemical properties, such as solubility and reactivity, which can influence their interaction with biological systems.

Summary

The analysis of features identified by XAI in relation to the toxicity of small molecules reveals several key insights. The presence of a heteroatom bonded to three oxygen atoms, such as in phosphate groups, is associated with increased chemical reactivity due to the electronegative nature of oxygen atoms,

potentially influencing toxicity (Alabugin et al., 2021). Tertiary amines, known for their nucleophilic properties, may interact with electrophilic sites in biological systems, contributing to toxicity (XpertAI, 2023). Additionally, carbon-oxygen single bonds, prevalent in functional groups like alcohols and ethers, can affect the solubility and reactivity of molecules, thereby impacting their toxicity (XpertAI, 2023). These features highlight the complex interplay between chemical structure and biological activity, underscoring the importance of understanding molecular interactions in toxicity predictions.

References

1. Alabugin, I. V., Kuhn, L., Medvedev, M. G., Krivoschapov, N. V., Vil', V. A., Yaremenko, I. A., Mehaffy, P., Yarie, M., Terent'ev, A. O., & Zolfigol, M. A. (2021). Stereoelectronic power of oxygen in control of chemical reactivity: the anomeric effect is not alone. *Chemical Society Reviews*.
2. XpertAI. (2024). XAI Summary.

Explanation generated with XpertAI (2024)

Understanding solubility of small molecules:

Features Identified by XAI Analysis

- Presence of an atom at an aromatic/non-aromatic boundary
- Presence of two heteroatoms bonded to each other
- Presence of an atom with three heteroatom neighbors

Presence of an atom at an aromatic/non-aromatic boundary:

Explanation: This feature is negatively correlated with solubility, as indicated by its strong negative correlation with SHAP values. The presence of such boundaries may affect the molecular planarity and symmetry, which are known to influence solubility.

Scientific Evidence: The SHAP analysis shows a strong negative correlation (correlation coefficient: -0.9531) with an average impact of 0.4801 (XpertAI, 2023). Additionally, disrupting molecular planarity and symmetry by eliminating aromaticity can enhance solubility (Ishikawa & Hashimoto, 2011).

Hypothesis: The presence of an atom at an aromatic/non-aromatic boundary reduces solubility by maintaining molecular planarity and symmetry, which are less favorable for solubility.

Presence of two heteroatoms bonded to each other:

Explanation: This feature also shows a strong negative correlation with solubility. The bonding of heteroatoms can influence the electronic distribution and hydrogen bonding potential, which are critical for solubility.

Scientific Evidence: The SHAP analysis indicates a strong negative correlation (correlation coefficient: -0.9688) with an average impact of 0.3475 (XpertAI, 2023). The presence of polar atoms like nitrogen or oxygen can alter solubility by affecting hydrogen bonding (Walker, 2017).

Hypothesis: The bonding of two heteroatoms may reduce solubility by altering the electronic distribution and reducing favorable hydrogen bonding interactions.

Presence of an atom with three heteroatom neighbors:

Explanation: This feature is negatively correlated with solubility, likely due to the complex electronic environment created by multiple heteroatom neighbors, which can affect solubility.

Scientific Evidence: The SHAP analysis shows a strong negative correlation (correlation coefficient: -0.9601) with an average impact of 0.2489 (XpertAI, 2023). The presence of multiple heteroatoms can influence solubility by affecting the molecule's electronic properties (Walker, 2017).

Hypothesis: An atom with three heteroatom neighbors may reduce solubility by creating an electronic environment that is less conducive to solubility.

Summary

The features identified by the XAI analysis, such as the presence of an atom at an aromatic/non-aromatic boundary, two heteroatoms bonded to each other, and an atom with three heteroatom neighbors, all show strong negative correlations with solubility. These features likely influence solubility by affecting molecular planarity, symmetry, electronic distribution, and hydrogen bonding potential. The presence of aromatic boundaries and heteroatom interactions can maintain

molecular structures that are less favorable for solubility, as supported by the SHAP analysis and literature on molecular modifications for solubility enhancement (XpertAI, 2023; Ishikawa & Hashimoto, 2011; Walker, 2017).

References

1. XpertAI. (2024). XAI Summary.
2. Ishikawa, M., & Hashimoto, Y. (2011). Improvement in Aqueous Solubility in Small Molecule Drug Discovery Programs by Disruption of Molecular Planarity and Symmetry.
3. Walker, M. A. (2017). Improvement in aqueous solubility achieved via small molecular changes.

Explanation generated with XpertAI (2024)

Understanding upper flammability limit of organic molecules:

Features Identified by XAI Analysis

- Structural Information Content Index (Neighborhood Symmetry of Zero-Order)
- Information Content Index (Neighborhood Symmetry of Order)
- Dipole Moment

Structural Information Content Index (Neighborhood Symmetry of Zero-Order)

Explanation: This feature quantifies the symmetry of a molecule's neighborhood at the zero-order level, which can influence how the molecule interacts with its environment, including its flammability characteristics.

Scientific Evidence: The document by Gharagheizi (2009) discusses the use of information index descriptors like SIC0, which account for neighborhood symmetry, in predicting the upper flammability limit (UFL) of organic compounds. An increase in SIC0 correlates with an increase in UFL (Gharagheizi, 2009).

Hypothesis: The Structural Information Content Index (Neighborhood Symmetry of Zero-Order) likely affects the UFL by influencing the molecular stability and reactivity, which are critical factors in determining flammability.

Information Content Index (Neighborhood Symmetry of Order)

Explanation: This feature is a generalized form of the previous index, focusing on the symmetry of molecular neighborhoods at various orders. It provides a broader perspective on molecular symmetry and its impact on flammability.

Scientific Evidence: The same study by Gharagheizi (2009) can be referenced here, as it discusses the role of information content indices in predicting UFL. The broader term "Information Content Index (Neighborhood Symmetry of Order)" would encompass various levels of symmetry, potentially offering a more comprehensive understanding of molecular interactions affecting UFL.

Hypothesis: The Information Content Index (Neighborhood Symmetry of Order) impacts the UFL by providing a detailed account of molecular symmetry, which influences how molecules interact with oxygen and other reactants during combustion.

Dipole Moment

Explanation: The dipole moment measures the separation of positive and negative charges within a molecule, affecting its polarity and interactions with other molecules, including those involved in combustion.

Scientific Evidence: While the provided documents do not explicitly discuss the dipole moment's impact on UFL, it is well-known in the literature that dipole moments can influence molecular interactions and stability, which are critical for flammability (Yuan et al., 2019).

Hypothesis: The dipole moment affects the UFL by altering the molecule's polarity, which can influence its reactivity and the energy required for combustion.

Summary

The features identified by the XAI analysis, including the Structural Information Content Index (Neighborhood Symmetry of Zero-Order), Information Content Index (Neighborhood Symmetry of Order), and Dipole Moment, all play significant roles in determining the upper flammability limit (UFL) of organic molecules. The Structural Information Content Index (Neighborhood Symmetry of Zero-Order) and its generalized form, Information Content Index (Neighborhood Symmetry of Order), quantify molecular symmetry, which influences molecular stability and reactivity. These factors can be crucial in determining how easily a molecule can ignite and sustain combustion. The dipole moment, although not explicitly discussed in the provided documents, could affect molecular interactions and stability, thereby influencing flammability. These features collectively provide a comprehensive understanding of the molecular characteristics that impact the UFL of organic compounds.

References

1. Gharagheizi, F. (2009). Prediction of upper flammability limit percent of pure compounds from their molecular structures. *Journal of Hazardous Materials*.
2. Yuan, S., Jiao, Z., Quddus, N., Kwon, J. S., & Mashuga, C. V. (2019). Developing Quantitative Structure-Property Relationship Models To Predict the Upper Flammability Limit Using Machine Learning. *Industrial & Engineering Chemistry Research*.

Explanation generated with XpertAI (2024)