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., Esrafili, 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. https://github.com/geemi725/XpertAI