



Metal-Organic Frameworks: Materials Modeling towards Engineering Applications

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Metal-organic frameworks (MOFs) have emerged as a new family of nanoporous materials. With an enormous choice of inorganic/organic building blocks, MOFs possess a wide range of surface area, pore size, and functionality and, thus, have been considered versatile materials for many potential applications. This book presents a broad collection of recent modeling studies in the field of MOFs toward potential engineering applications, such as gas storage/separation, carbon capture, catalysis, water purification, and drug delivery. The subject of this book renders it unique, for while the various topics on MOFs boast vast literature, there is not yet a single coherent collection for modeling endeavors. The book will appeal to scientists, engineers, and students in the multidisciplinary intersections of materials science, chemistry, and engineering.

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