AUGMENTING THE ADSORPTION MECHANISMS IN METAL-ORGANIC FRAMEWORKS VIA *IN Silico* METHODS

By

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Metal-organic frameworks (MOFs), intricate structures composed of organic linkers and metal nodes, exhibit remarkable versatility with applications ranging from gas adsorption and separation to drug and energy storage, water absorption, and catalysis. Despite their broad utility, a comprehensive understanding of the factors influencing adsorption within MOFs is essential for optimizing their potential as adsorbents. This study systematically categorizes and investigates various factors through computer simulations, shedding light on their nuanced effects.

The first focus centers on the functionalization of IRMOF-74-III with amine groups, a critical aspect of enhancing drug adsorption. The exploration delves into the impact of different numbers and positions of amine functional groups on the MOF's behavior, utilizing density functional theory (DFT) and molecular docking. As the number of amine group increases, the MOF's pore polar surface area expands, but a reduction in the energy gap between the HOMO and LUMO orbitals is observed. Electrostatic potential contours reveal distinct pockets on the amine-functionalized IRMOF-74-III's pore wall, which fenbufen@MOF showing the most stable drug@MOF complex. The study emphasizes the crucial role of unsaturated magnesium sites in frameworks and specific functional groups on drugs for interactions and charge transfer. The second exploration addresses MOFs' ability to selectively adsorb isomers, as exemplified by MIL-53(Al) MOF's adsorption of xylene isomers. The introduction of non-polar functional groups on the organic linker was proposed for enhanced adsorption. Computational analysis of different configurations of dimethyl-functionalized phenyl rings reveals *meta*-dimethyl-MIL-53(Al) (MDM) as an optimal structure for xylene adsorption, demonstrating superior adsorptive separation of *ortho*- over *meta*- and *para*-xylene. The third study introduces an innovative alternative to MOF functionalization by directly replacing the organic linker with a structurally similar compound, preserving the framework topology. Using computer simulations, the impact of replacing the organic linker in HKUST-1 MOF with borazine is analyzed. Borazine-based HKUST-1(Cu) (hB-HKUST-1(Cu)) exhibits a significant improvement in CO_2 adsorption compared to the conventional

MOF, with the adsorption primarily governed by framework-gas interactions between CO_2 and the boron atom in borazine. Lastly, scalability which is a crucial factor for large-scale applications is addressed through the evaluation of CALF-20 (Zn) MOF. While its ability to adsorb CO_2 is already established, its performance with other gases remains uncertain. GCMC and MD simulations reveal CALF-20 (Zn) as a potential MOF for selectively adsorbing polar and non-polar toxic gases, emphasizing its applicability in diverse scenarios.

In conclusion, this comprehensive study utilizes atomic-level details obtained through computer simulations to elucidate several underexplored factors in MOF adsorption. The insights gained from optimizing drug adsorption in IRMOF-74-III to enhancing selectivity for xylene isomers in MIL-53(Al) and improving CO_2 adsorption in HKUST-1, will contribute significantly towards advancing the design and application of MOFs in gas adsorption for various industrial scenarios.

Keywords: Adsorption; Metal-Organic Framework; Molecular Simulations

SDG: GOAL 3: Good Health and Well-Being; GOAL 4: Quality Education

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia
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MENAMBAHBAIK PENJERAPAN DALAM STRUKTUR LOGAM-ORGANIK MELALUI KAEDAH SIMULASI KOMPUTER

Oleh

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Rangka kerja logam-organik (MOF) iaitu struktur rumit yang terdiri daripada penghubung organik dan nod logam, mempamerkan kepelbagaian yang luar biasa dengan aplikasi daripada penjerapan dan pengasingan gas kepada penyimpanan ubat dan tenaga, penyerapan air dan pemangkinan. Walaupun kegunaannya yang luas, pemahaman menyeluruh tentang faktor-faktor yang mempengaruhi penjerapan dalam MOF adalah penting untuk mengoptimumkan potensi mereka sebagai penjerap. Kajian ini secara sistematik mengkategorikan dan menyiasat pelbagai faktor melalui simulasi komputer, menjelaskan kesannya yang terselindung.

Kajian awal tertumpu pada pefungsian IRMOF-74-III dengan kumpulan amina, suatu aspek kritikal dalam meningkatkan penjerapan ubatan. Penerokaan ini melihat kepada kesan nombor dan kedudukan yang berbeza kumpulan berfungsi amina terhadap perilaku MOF, menggunakan teori fungsian ketumpatan (DFT) dan pendokkan molekul. Apabila bilangan kumpulan amina bertambah, kawasan permukaan berkutub pori MOF mengembang, tetapi didapati terdapat pengurangan dalam jurang tenaga antara orbital HOMO dan LUMO. Kontur keupayaan elektrostatik mendedahkan beberapa poket yang berbeza pada dinding pori IRMOF-74-III yang telah difungsi dengan amina, yang mana fenbufen@MOF menunjukkan kompleks ubat@MOF yang paling stabil. Kajian ini menekankan peranan penting tapak tak tepu magnesium dalam rangka kerja dan kumpulan berfungsi spesifik terhadap ubat bagi tujuan interaksi dan pemindahan caj. Penerokaan kedua menangani keupayaan MOF untuk menjerap isomer secara selektif, seperti yang ditunjukkan oleh penjerapan isomer xilena MIL-53(Al) MOF. Pengenalan kumpulan berfungsi tak berkutub pada penghubung organik dicadangkan untuk mempertingkatkan penjerapan. Analisis pengkomputeran bagi konfigurasi berbeza cincin fenil terfungsi-dimetil mendedahkan *meta*-dimetil-MIL-53(Al) (MDM) sebagai struktur optimum bagi penjerapan xilena, yang menunjukkan pemisahan penjerapan unggul bagi *orto*- yang melampaui *meta*- dan *para*-xilena. Kajian ketiga memperkenalkan alternatif inovatif kepada kefungsian MOF dengan menggantikan secara terus penghubung organik dengan sebatian yang serupa dari segi struktur, yang

memelihara topologi rangka kerja. Menggunakan simulasi berkomputer, kesan terhadap penggantian penghubung organik dalam MOF HKUST-1 dengan borazina telah dianalisis. HKUST-1(Cu) yang berasaskan borazine (hB-HKUST-1(Cu)) mempamerkan peningkatan ketara dalam penjerapan CO_2 berbanding MOF konvensional, dengan penjerapan terutamanya dikawal oleh interaksi rangka kerja-gas, iaitu antara CO_2 dan atom boron dalam borazina. Akhir sekali, kebolehskalaan yang merupakan faktor penting untuk pengaplikasian berskala besar dijawab melalui penilaian MOF CALF-20 (Zn). Walaupun keupayaannya untuk menyerap CO_2 telah pun nyata, prestasinya dengan gas lain masih tidak ditentukan. Simulasi GCMC dan MD mendedahkan CALF-20 (Zn) sebagai MOF yang berpotensi untuk menjerap gas toksik berkutub dan tak berkutub secara selektif, menonjolkan lagi kebolehannya untuk digunakan dalam pelbagai senario.

Kesimpulannya, kajian komprehensif ini menggunakan butiran di peringkat atom yang diperoleh melalui simulasi berkomputer untuk menjelaskan beberapa faktor yang kurang diterokai dalam penjerapan MOF. Pengetahuan yang diperoleh daripada mengoptimumkan penjerapan ubat dalam IRMOF-74-III kepada meningkatkan selektiviti untuk isomer xilena dalam MIL-53(Al) dan menambah baik penjerapan CO_2 dalam HKUST-1, akan sangat menyumbang kepada kemajuan reka bentuk dan aplikasi MOF dalam penjerapan gas untuk pelbagai senario industri.

Kata kunci: Jerapan; Rangka kerja Logam-Organik; Simulasi Molekul

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°C	Celsius
μ	electronic chemical potential
μm	micrometres
1D	one dimensional
^{1}H NMR	proton nuclear magnetic resonance
^{27}Al NMR	aluminum nuclear magnetic resonance
2D	two dimensional
3D	three dimensional
5-FU	5-fluorouracil
Å	angstrom
Å^{2}	square angstrom
Å^{3}	cubic angstrom
AD	average distance
Al	Aluminium
$AlCl_3 \cdot 6H_2O$	aluminum chloride hexahydrate
AM1	Austin Model 1
Asp	aspirin
atm	atmosphere
B3LYP	Becke three-parameter Lee-Yang-Parr
BDC	1,4-benzenedicarboxylate
BET	Brunauer-Emmett-Teller
BN-MOFs	borazine-based metal-organic frameworks
$bphdcH_2$	benzophenone-4,4′-dicarboxylic acid
BPNN	back-propagation neural network

Bq	ghost atoms
Br	bromo functional group
btc	1,3,5-benzene tricarboxylate
C_4H_4	buta-1,3-diene functional group
C_8H_{10}	xylene
Caf	caffeine
CALF-20	Calgary Framework 20
CB-GCMC	Configurational Bias Grand Canonical Monte Carlo
CCDC	cambridge crystallographic data center
CD	closest distance
CH_3	methyl functional group
$CH_3)_2$	dimethyl functional group
CHELPG	CHarges from ELectrostatic Potentials using a Grid-based method
cif	crystal information file
$Cl)_2$	dichlorine functional group
Cl_2	chlorine gas
C_m	carbon atoms of the methyl group
$cm^2.s^{-1}$	square centimeter per second
$cm^3.g^{-1}$	gram per cubic centimetre
C-MOF	carbon-based metal-organic frameworks
CNTs	carbon nanotubes
CO	carbonyl functional group
Co	Coblt
CO_2	carbon dioxide
COFs	covalent organic frameworks

C_p	carbon atoms of phenyl ring
CP	closed pore form
CS_A	chemical shift anisotropic
CSGT	continuous set gauge transformations
CS_I	chemical shift isotropic
Cu	Copper
CUSs	coordinatively unsaturated sites
D	dipole moment
DFT	density functional theory
DMAc	N,N-dimethylacetamide
DMF	dimethylformamide
DOS	density of states
DPNI	N,N'-di-(4-pyridyl)-1,4,5,8-naphthalenetetracarboxydiimide
drug@MOFs	drug molecule complexed in metal-organic frameworks
D_s	self-diffusion coefficient
e.g.	for example
E+G	sum of electronic and thermal free energies
E+H	sum of electronic and thermal enthalpies
E+T	sum of electronic and thermal energies
E_0	ground state energy
EA	electron affinity
E_{ad}	adsorption energy
$E_{complex}$	total energy of complex system
E_{corr}	correlated movement of electrons of different spin
E_{coul}	classical electron-electron coulomb repulsion energies

E_{exch}	non-classical electron-electron exchange energies
E_{gap}	energy gap
E_{ij}	stabilization energies
EMD	equilibrium molecular dynamics
EMIL-53(Al)	total energy of MIL-53(Al)
E-MOF	energetic MOFs
E_{NN}	repulsion energy between nucleuses
E_{PR}	electron paramagnetic resonance
ESP	electrostatic potential
E_T	kinetic energy of the electrons
etc	et cetera or other similar things
EV	attraction energy between nucleus and electron
eV	electronvolt
E_{xylene}	total energy of xylene
ε	well depth
ε_0	permittivity of free space
F_2	fluorine gas
Fe	Iron
Fen	fenbufen
FMOs	frontier molecular orbitals
fs	femtosecond
g(r)	distribution of particles
$g.g^{-1}$	gram per gram
GAFF	general amber force field
GCMC	grand canonical monte carlo

Gem	gemcitabine
GIAO	Gauge-independent atomic orbital
$\hat{H}$	hamiltonian operator
H_2	hydrogen gas
H_2BDC	1,4-benzenedicarboxylic acid
$H_2BDC\text{-}(CH3)_2$	2,5-dimethyl terephthalic acid
H_2DTDAO	dibenzo[b,d]thiophene-3,7-dicarboxylic acid 5,5-dioxide
H_2FDCA	9-fluorenone-2,7-dicarboxylic acid
H_2O	water
H_2S	hydrogen sulfide gas
H_3BTC	1,3,5-benzenetricarboxylic acid
H_6TDPAH	2,5,8-tris(3,5-dicarboxylphenylamino)-s-heptazine acid
HB	hydrogen bond interactions
H-BEA	protonic beta zeolite
hB-HKUST-1	borazine-based HKUST-1
He	helium
Hep	heparin
HF	hartree-fock theory
HKUST	Hong Kong University of Science and Technology
H_m	hydrogen atoms of the methyl group
HME	protonated melamine
HOMO	the highest occupied molecular orbital
H_p	hydrogen atoms of the phenyl ring
H-Y	H-type of zeolite Y
IAST	ideal adsorbed solution theory

Ibu	ibuprofen
IDLH	immediately dangerous to life or health
IITKGP	Indian Institute of Technology Kharagpur
Imt	imatinib
IP	ionization potential
IPM	IISER Pune Materials
K	Kelvin
$kg.m^{-3}$	kilogram per cubic metre
K_H	Henry coefficient
$kJ.mol^{-1}$	kilojoule per mole
kPa	kilopascal
LGA	Lamarckian genetic algorithm
LJ	Lennard-Jones
LMCT	ligand to metal charge transfer
LP	Lone electron pair
LP*	unfilled valence-shell nonbonding
LUMO	the lowest unoccupied molecular orbital
$m^2.g^{-1}$	square meter per gram
mbar	millibar
MC	monte carlo
MD	molecular dynamics
MDM	meta-dimethyl functionalized-MIL-53(Al)
MEP	molecular electrostatic potential
Mg	magnesium
$mg.g^{-1}$	milligrams per gram

MIL-53	Materials of Institute Lavoisier 53
ML	machine learning
MM	molecular mechanics
MMMs	mixed-matrix membranes
$mmol.g^{-1}$	milligram per gram
MNDO	modified neglect of differential overlap
MOFs	metal-organic frameworks
$mol.kg^{-1}$	mole per kilogram
MS	magnetic susceptibility
MSD	mean square displacement
MTX	methotrexate
MVT-MOFs	multivariate metal-organic frameworks
mx	*meta*-xylene
N	number of particles
N_2	nitrogen gas
Nap	naproxen
NBO	natural bond orbital
NEMD	non-equilibrium molecular dynamics
NH_2	amino functional group
NICS	Nucleus-Independent Chemical Shifts
nm	nanometer
nm^2	square nanometer
NMR	nuclear magnetic resonance
NO	nitrogen monoxide
NO_2	nitro functional group

NPT	constant number of particles, pressure and temperature
ns	nanosecond
NSAIDs	non-steroidal anti-inflammatory drugs
NTTA	5,5′,5″-((4,4′,4″-nitrilotris(benzoyl))tris-(azanediyl))triisophthalic acid
NVE	constant number of particles, volume and energy
NVT	constant number of particles, volume and temperature
$OC_3H_5)_2$	dipropoxy functional group
$OC_7H_7)_2$	benzyloxy functional group
OCH_3	methoxy functional group
ODM	*ortho*-dimethyl functionalized-MIL-53(Al)
OH	hydroxyl group
Ori	Oridonin
ox	*ortho*-xylene
PAAS	poly (acrylic acid) sodium
PBC	periodic boundary conditions
PBDA	4,4'-((2-(tert-butyl)-1,4-phenylene)bis(oxy))dibenzoic acid
PDM	*para*-dimethyl functionalized-MIL-53(Al)
PET	polyethylene terephthalate
PM3	method number 3
PM6	parametric method number 6
PPD	*para*-phenylenediamine
ppm	parts per million
PPX	porous metallocavitand pillarplex
PSD	pore size distribution
PSM	post-synthetic modification

px	*para*-xylene
Q	charge
QENS	quasi-elastic neutron scattering
Qeq	charge equilibration
QM	quantum mechanics
QM/MM	quantum mechanics/molecular mechanics
Q_{max}	adsorption capacities
QSAR	quantitative structure-activity relationship
Q_{st}	heat of adsorption
R	ideal gas constant
RACs	revised autocorrelations
RDF	radial distribution function
r_i	center-of-mass of the particle i
S	entropy
S	sulfur
SBUs	secondary building blocks
SO_2	sulfone
SO_2	sulfur dioxide gas
SO_3H	sulfonic functional group
sod	sodalite topology
SPXRD	synchrotron powder X-ray diffraction
sql	square lattice topology
S_s	chemical softness
Ssp	sorbent selection parameter
STY	space-time yield

T	temperature
t	time
Tam	Tamoxifen
TEMPO	2,2,6,6-Tetramethylpiperidin-1-yl)oxyl
TG	thermal gravimetric
TGA	thermogravimetric analysis
TPSA	topological polar surface area
TraPPE	Transferable Potentials for Phase Equilibria force field
U	total energy
UiO	Universitetet i Oslo
V	Vanadium
v	volume
VOCs	volatile organic compounds
VSA	vacuum swing adsorption
VT-PXRD	variable-temperature powder x-ray diffraction
W^{IG}	ideal-gas Widom Rosenbluth weight
wt%	weight percent
ZDO	Zero differential overlap
ZIFs	zeolite imidazolate frameworks
ZJNU	Zhejiang Normal University
Zn	Zinc
Zn-Atz	Zinc-aminotriazolato-oxalate
Zr	Zirconium
ZU	Zhejiang University
α	ntrinsic thermodynamic selectivity

α	polarizability
η	global hardness
μ_3-OH	bridging hydroxyl groups
ρf	density
σ	diameter
σ_h	horizontal plane of molecules
χ	electronegativity
Ψ	wavefunctions
ω	electrophilicity

CHAPTER 1

INTRODUCTION

1.1 Metal-Organic Frameworks (MOFs)

Porous materials such as activated carbon, zeolites, silica gel, covalent-organic frameworks (COFs), and metal-organic frameworks (MOFs) have a structure that contains interconnected voids or pores, which can be of various sizes and shapes (Bennett et al. 2021). These types of materials can absorb and hold liquids, gases, or even other solid particles within their pores. Nanoporous materials are a specific class of materials that possess a network of pores or voids on a nanometer scale (typically with pore sizes less than 100 nanometers) (Thommes et al. 2021).

MOFs are crystalline solid materials and they are made up of inorganic nodes and organic linkers (James 2003). MOFs are given as one- (1D), two- (2D) and three- (3D) dimensional porous networks. MOF materials emerged in the late 1980s and they became a major field of research for many potential applications at the end of the 1990s (Cook et al. 2012). A great degree of unique features such as large surface area, tunable pore size, high thermal and chemical stability, recyclability and diversity of structures have been distinguished for MOFs (Cook et al. 2012). These advantages have offered a wide range of industrial processes including gas storage and separation, energy storage, wastewater treatment, catalysis and drug storage (Silva et al. 2015). Some MOFs are shown to be high-potential adsorbents compared to the conventional materials (Khan et al. 2013). As an example of conventional materials, carbon nanotubes (CNTs) which are frequently used for drug adsorption, are still encountered with controlling the pore size (Song et al. 2017). Moreover, activated carbon is an inexpensive, non-toxic material and it can be obtained from natural carbon resources (Miriyala et al. 2017). Activated carbon materials have large surface area and great adsorption ability through non-covalent interactions with gas molecules, however, these interactions cannot provide high selectivity for gas adsorption. Also, large pores and open gates in mesoporous silica M41S materials have made the possibility for receiving large-size guest molecules (Linares et al. 2014). However, the use of mesoporous silica M41S materials has become restricted due to a lack of high catalytic activity and hydrothermal stability. In another example, zeolites are taken advantage of long-term chemical and biological stability, but the capability of zeolites has been limited because of their small pore size and poor structural diversity (Reeve et al. 2018).

1.2 Adsorption Mechanisms in MOFs

MOFs constitute a versatile class of porous materials with diverse pore sizes, including mesoporous, microporous, and ultra-microporous structures. The stability and applications of MOFs are intricately linked to their unique porous architectures. In the case of mesoporous MOFs, characterized by pore sizes ranging from 2 to 50 nm, their structural stability often stems from the judicious choice of metal nodes and organic

linkers (D. Liu et al. 2018). These materials exhibit enhanced stability compared to traditional porous materials, facilitating applications such as gas storage, catalysis, and drug delivery. The mesoporous nature allows for the accommodation of larger guest molecules, contributing to their utility in diverse fields. Moving to microporous MOFs, which possess pore sizes typically below 2 nm, their stability is often attributed to the precise control of the framework's topology (Lin et al. 2020a). The smaller pore dimensions create a confinement effect, influencing the adsorption and diffusion properties of guest molecules. This structural control enhances stability and leads to applications in gas separation, sensing, and selective catalysis. Microporous MOFs have shown promise in efficiently capturing specific gases, a critical aspect in environmental and industrial contexts. Ultra-microporous MOFs, with pore sizes below 1 nm, represent a frontier in the design of porous materials (Adil et al. 2017). Achieving stability at such diminutive scales requires advanced synthetic strategies and a deep understanding of intermolecular interactions. These ultra-microporous MOFs exhibit exceptional stability under various conditions, paving the way for applications in sieving small molecules and separation processes at the molecular level. Their potential applications span fields such as molecular recognition, chiral separation, and membrane technology.

The adsorption in MOFs can be categorized into several types based on the size of the adsorbates and the nature of the interactions between the MOF and the adsorbate molecules. Some common types of adsorptions in MOFs include the adsorption of small gas molecules, drug molecules, and liquids (Gonzalez-Hernandez et al. 2021). MOFs can be designed to selectively adsorb small molecules, such as carbon dioxide, methane, or volatile organic compounds (VOCs), which are relevant to environmental and gas storage applications. The advantages of using MOFs for drug adsorption and delivery include enhanced drug stability, prolonged release kinetics, and the ability to target specific tissues or cells (Wu and Yang 2017). The porous nature of MOFs allows for high drug-loading capacities, which can reduce the frequency of drug administration. Furthermore, the tunability of MOFs allows researchers to design materials with tailored drug release profiles. Applications of liquid adsorption in MOFs are mainly included water, alcohols, and organic solvents (Li et al. 2017). However, it's important to note that not all MOFs are suitable for liquid adsorption, as some may be unstable in the presence of certain liquids or exhibit limited adsorption capacities (De Toni et al. 2012). The selection of the appropriate MOF for a specific liquid adsorption application requires careful consideration of the MOF's properties and the characteristics of the target liquid.

There are two main mechanisms that have been observed for MOF adsorption, which are via physisorption and chemisorption. Physisorption, also known as physical adsorption or van der Waals adsorption, occurs when weak forces such as London dispersion forces or dipole-dipole interactions between the adsorbate molecules and the MOF surface led to adsorption (Ramanayaka et al. 2019). Physisorption is usually reversible, and the adsorbate can be released easily by reducing the pressure or increasing the temperature. In terms of cyclability, physisorption is generally characterized by its ease of desorption, making it a reversible process. The weak nature of the interactions allows the adsorbed molecules to be released from the material surface under mild conditions, facilitating multiple cycles of adsorption and desorption without significant deterioration of the material. The bond formation results in more stable adsorption, but it also tends to make the process less reversible. Chemisorption is typically associated with a higher energy barrier for desorption, leading to decreased cyclability compared to physisorption.

Chemisorption, or chemical adsorption, involves stronger chemical bonds between the adsorbate molecules and the MOF surface (Ramanayaka et al. 2019). This results in a more stable and irreversible adsorption process. Chemisorption can occur through processes like covalent bonding, coordination bonding, or metal-ligand interactions, depending on the specific MOF structure and the nature of the adsorbate.

1.2.1 Factors that affect adsorptions in MOFs

Adsorptions in MOFs are governed by different factors such as surface area, pore volume, interpenetration, size and shape of pore gate, chemical compositions, functionalization, topology, coordinatively unsaturated sites (CUSs), and flexibility. In addition, some properties of adsorbates including molecular size and shape, polarity, and molecular weight are influential towards the adsorption performance in MOFs.

The effect of CUSs and surface area was highlighted in a combined experimental and computational study. A cancer drug imatinib (Imt) was found to have better adsorption in MIL-101(Cr) compared to MIL-100(Fe) (MIL stands for Materials of Institute Lavoisier) (Qi et al. 2016). The binding energy for Imt@MIL-101(Cr) and Imt@MIL-100(Fe) complex systems was obtained as -9.90 and -9.17 kcal.mol^{-1}, respectively. The presence of unsaturated Cr(III) and Fe(III) in the frameworks led to strong interactions with Imt. The surface area of MIL-101(Cr) is larger (3311.88 m^2.g^{-1}) than MIL-100(Fe) (1225.53 m^2.g^{-1}) which contribute to better adsorption. MOF's surface area and stability can be enhanced when the frameworks are interpenetrated. Interpenetration in MOFs, same as other materials, occurs naturally when two or more networks are nested within each other's pore spaces. Many researches have reported that interpenetration in MOFs can enhance the rate of adsorption of small gas molecules by giving an optimal pore size and stronger interactions (Elsaidi et al. 2014) (Lin et al. 2020b).

The size and shapes of the MOFs' wall surface as well as the pore gate have been shown to determine the adsorptive performance. It was found that the V-shaped clefts in the MOF $[Zn(BDC)(H_2O)_2]_n$ were selective towards drug molecules (Rodrigues et al. 2012). Ibuprofen and methylene blue fit entirely inside the clefts and made strong interactions with the coordinated zinc (Zn) metal in addition to weak π-π interactions with phenyl rings in the frameworks. However, gentamicin and amoxicilin did not fit into the V-shaped clefts due to their larger molecular size. Some MOFs are made up of different types and sizes of pore windows. For example, MIL-101 have triangular (6 Å), pentagonal (12 Å), and hexagonal (15 Å) pores in its framework. Yang and colleagues found that MIL-101 pore windows had selective adsorption toward xylene isomers, favoring the *para*-xylene isomer (K. Yang et al. 2011).

MOFs exhibit remarkable diversity when it comes to their topological features. These arise from the combination of metal nodes and organic linkers, resulting in a vast array of frameworks with varying pore sizes, shapes, and connectivity. Tuning the pore topological features allows for positioning optimal adsorption sites within the framework. Having the appropriate topology enables the MOF to be an energy-efficient adsorbent (Anderson et al. 2018). An energy-efficient adsorbent refers to a material that

possesses characteristics enabling it to effectively capture and release guest molecules with minimal energy input. The topology of MOFs can be tailored to have specific pore sizes and geometries. This tunability allows for selective adsorption of molecules based on their size and shape. Selectivity minimizes the energy spent capturing unwanted molecules and enhances the efficiency of the adsorption process. The knowledge that the topology of MOFs can be tailored to have specific pore sizes and geometries, leading to tunability and selective adsorption of molecules, is well-established in the field of porous materials and has been extensively studied and documented in the scientific literature. For example, a hexagonal tube-shaped MOF, $[Zn(\mu_4\text{-L})]_n$ (Zn-MOF), having a rare topology of **ptr** experienced selective adsorption of *para*-xylene over its *ortho*- and *meta*- counterparts at higher pressure (Huang et al. 2015). In another study, 38 polymorphic MOFs were extensively applied for the adsorption of linear and branched C4-C6 alkane isomers (Bobbitt, Rosen, and Snurr 2020). It was discovered that MOFs having small pore and **nbo** topology had a high affinity for linear alkanes, while the frameworks were deprived to uptake of the branched alkanes.

There are isostructural MOFs that have similar chemical structures but different chemical compositions. To improve certain functionality of MOFs, the conventional carbon-based organic linkers can be replaced with nitrogen (N)-, oxygen (O)- and sulfur (S)-rich organic linkers. Although the presence of the heteroatoms such as N, O, and S in organic linkers can cause deviation from the straight and rigid shape of the linker, the overall desired crystal structure of the MOF can still be obtained (Hu et al. 2018a) (Hu et al. 2018b). N-rich MOFs are well-known as energetic MOFs (E-MOF) and they have high heat denotation, high density, impact-insensitive, and good thermostability (Q. Liu et al. 2016). O-rich MOFs are exceptionally stable in aqueous solutions, highly sensitive to metal ions, and excellent chromophores to absorb light energy (L. Liu et al. 2018). S-rich MOFs have the advantage of high conductivity (Wu et al. 2020) and electrochemical performance (M.-T. Li et al. 2018). Altogether, the presence of N-, O- and S-rich organic linkers resulted in promoting the interaction sites and subsequently greater adsorption.

MOF crystal lattices can be functionalized with chemical groups for the purpose of boosting their performance for adsorption and separation. Based on the target framework and chemical groups, functional groups can be incorporated on organic linkers, grafted on CUSs, or coated on the MOF's crystal surfaces. The use of amide-functionalized MOFs for gas storage and separation was reviewed by Bai *et al*. (Xue, Wang, and Bai 2019). It was stated that owing to the intrinsic nature of amide functional groups such as flexibility and polarizability, a wide variety of topologies for amide-functionalized MOFs were reported which were promising for gas adsorption and separation.

There have been reported that some influential factors could contribute towards higher CH_4 adsorption in MOFs such as electrostatics, van der Waals forces, and MOF flexibility (Petit 2018). A unique feature of MOFs is the potential flexibility of the framework which is governed by temperature, pressure, oxidation number of metals and length of organic linkers. Nevertheless, the flexibility of MOFs is not noticeable in the solvent because solvent molecules fill the pores (Van de Voorde et al. 2014). MIL-53 is the common type of MOF that has demonstrated efficient flexibility on gas adsorption, while its isostructure MIL-47 has an almost rigid pore. In 2011, Clet *et al*. detected the reason for less flexibility in MIL-47(V) by using the activation method in order to yield

MIL-47(V^{IV}) and MIL-47(V^{III}) (Leclerc et al. 2011). They declared that MIL-47(V^{III}) had μ_2-hydroxyl groups (as the analogous structure MIL-53) which provided a higher flexible framework compared to MIL-47(V^{IV}). In the presence of H_2O and CO_2, the hydroxyl group became the most favorable adsorption site for the adsorbates.

1.3 Computer Modeling of MOFs

Computer modeling is one of the most fascinating techniques in chemistry that combines theoretical aspects with the use of high-performance computers and software packages (Almeida et al. 2017). The possibility of atomistic observation in detail such as interactions and charge density distributions of molecules can be provided by computer modeling that is not simply available via experimental equipment. Molecular modeling and simulations can provide a cost-effective and efficient way to gain a deeper understanding of MOF functionalization. This eliminates the need for every potential functionalized MOF to be successfully synthesized. They can complement experimental efforts and guide the design of novel functionalized MOFs with improved performance in various practical applications. Researchers can perform high-throughput screening to identify promising candidates for further experimental testing. Furthermore, molecular simulations aid in determining the most suitable locations for functional groups within the MOF structure. By studying various configurations, researchers can identify the positions that lead to the highest adsorption capacities or specific binding sites for target molecules. Computer modeling and simulations involving MOF structures are mainly divided into two groups; i) quantum mechanics (QM) to characterize the MOF crystal structures and ii) molecular mechanics (MM) to find appropriate MOF structure for a desired application (Kotzabasaki et al. 2018). MM-based methods commonly consist of docking, grand canonical monte carlo (GCMC) and molecular dynamics (MD) simulations. Computer modeling strategies also have been shown capable and valuable in designing new MOFs (hypothetical MOF) structures for very specific targeted properties (Demir et al. 2023).

1.3.1 Density Functional Theory (DFT)

DFT calculations are widely used to study the electronic structure, properties, and behaviour of MOFs. DFT is a quantum mechanical approach that models the electronic properties of a system based on the electron density distribution rather than solving the Schrödinger equation directly for each electron. It provides a powerful and efficient method for understanding the behavior of MOFs at the atomic and electronic levels. Experimental validation and comparison with other theoretical methods are carried out to ensure the accuracy and reliability of the DFT methods and algorithms. DFT calculation for MOFs usually consists of geometry optimization, determining the basis set and pseudopotentials, building unit cells and supercells, as well as electronic structure analysis. For example, DFT calculations were used to analyze the adsorption mechanism of H_2S, SO_2 and SF_6 on MOF-505 analogue (Li et al. 2021). Based on the analyzing adsorption energy and binding distance, density of states (DOS), charge transfer, charge densities and electron localization function, selectivity relationship of organic ligands and metal sites was $SO_2 \geq H_2S > SF_6$. The adsorptions of SO_2 and H_2S were occurred via chemical adsorption, thus the MOF-505 analogue can be better adsorbent for fault

recovery of SF_6 circuit breaker. In another study, DFT optimization elucidated changes in electronic properties of MOF-5 after its doped variants (M@MOF-5, M = Co, Fe, Ni and Mn) (Panda et al. 2022). The results suggested that unoccupied *d* orbitals on the dopants caused reducing of the band gap and the ligand to metal charge transfer (LMCT) in M@MOF-5. The existence of more empty *d* orbitals along with easy LMCT gave rise to the narrowest band gap in Fe@MOF-5 as it nominated for a promising visible-light-driven photocatalyst.

1.3.2 Grand Canonical Monte Carlo (GCMC)

GCMC simulations are a powerful computational technique that can be used to study the adsorption and desorption of molecules in porous materials like MOFs. The simulations are carried out in the grand canonical ensemble, where the number of adsorbate molecules, the volume of the system, and temperature are allowed to fluctuate, while the chemical potential is fixed. The simulations aim to calculate various properties, such as adsorption isotherms, adsorption heats, and diffusion coefficients, providing valuable insights into the MOF's gas adsorption behavior and performance. GCMC simulations for MOFs involve modeling the adsorption process of adsorbate molecules into the MOF structure at a given temperature, pressure, and chemical potential. As an example, the adsorption capacity of HKUST-1 and MIL-101 for CH_4 and CO_2 gases was explored by GCMC simulation were found to be consistent with the experimental data within 5-10% error ranges (Teo, Chakraborty, and Kayal 2017). As a result, two distinct types of adsorption sites were identified: van der Waals potential pore sites with dispersive interactions and CUSs with Coulomb attraction. By analyzing experimental and hypothetical heat of adsorption (Q_{st}) data, it was determined that HKUST-1 was very micro-porous and possessed high Coulomb attractions towards adsorptive molecules. The unique structural features of HKUST's micropores contribute to increased surface area and adsorption interactions and, consequently, higher heats of adsorption. In another literature, GCMC was utilized for study of adsorption and separation behaviors of pure CO_2 and mixture CO_2/N_2 in three MOFs; MOF-5, MOF-74 and ZIF-8 (Tao, Zhang, and Xu 2022). The authors observed that MOF-5 had the highest saturation adsorption capacity for pure CO_2 (35 $mmol.g^{-1}$) at room temperature, whereas MOF-74 showed the highest CO_2 uptake (11 $mmol.g^{-1}$) under 10 bar. Also, the selectivity of CO_2 over N_2 in MOF-74 was found to be the highest, approximately 38, because of the strongest binding force with CO_2.

1.3.3 Molecular Dynamics (MD)

MD simulations are another widely used computational technique for studying the behaviour of molecules in MOFs. MD simulations allow for the dynamic evolution of the MOF system over time, providing valuable insights into its structural stability, thermal properties, and molecular interactions. In MD simulations for MOFs, the MOF structure and adsorbate molecules are treated as a collection of atoms whose positions and velocities are propagated forward in time according to the laws of classical mechanics. The interactions between the atoms are described by a force field, which includes bonded and non-bonded interactions such as covalent bonds, van der Waals forces, and electrostatic interactions. MD simulations well employed for study of

dynamics behavior of MOF frameworks during adsorption process. For instance, rotational and the translation mobility of xylene isomers adsorbed in MOF-5 was explored by nuclear magnetic resonance (NMR) spectroscopy and MD simulations (Witherspoon et al. 2017). The experiments showed that for the *para*-, *meta*-, *ortho*-, xylene isomers, the translational motion activation energies were 15.3, 19.7, and 21.2 $kj.mol^{-1}$ and the rotational motion activation energies were 47.26, 12.88, and 11.55 $kj.mol^{-1}$, respectively. So, *para*-xylene indicated faster transitional motion than other isomers. The results obtained from MD simulations confirmed that *para*-xylene had the lower free energy barrier for hopping away from its binding sites. The presence of inter-crystalline space is demonstrated to have significant influence on the adsorption, structure, and dynamics of the adsorbed fluid, although most molecular simulation studies rely on perfect single-crystal models of MOF materials (Gautam and Cole 2020). In a recent study assisted by MD simulation, Dhiman and colleagues found the relationship between single-crystalline space and adsorption sites in Mg-MOF-74 (Dhiman et al. 2023). They found that wider inter-crystalline spacing, anomalous loading was depended on the translational diffusivity of CO_2. Also, inter-crystalline spacing suppresses the rotational motion of CO_2.

1.4 Problem Statement and Hypothesis

Although many factors have been identified to influence the adsorption in MOFs, several are still not thoroughly studied. The functionalization of organic linkers has been studied extensively in the past years. This is because the functionalization of MOF's organic linker can significantly promote adsorption (Razavi and Morsali 2019a). However, there are still many gaps in the understanding of the effect of varying the functionalization sites or the number of groups. For example, although amine functionalization on organic linkers has been extensively studied, the effect of increasing the number of amine groups on drug adsorption has not been elucidated. The works on a single amine group (Xu and Yan 2016a) and two groups (*para*) functionalization (Leo et al. 2019a) on phenyl ring have never been compared before. Functionalizing with diamine ($-2NH_2$) groups on organic linkers allows for *ortho*, *meta* and *para* isomerism. These sets of amine-functionalized linkers may generate different electronic and dynamic conditions on the MOF's pore wall, assuming the overall framework topology is unaffected. There is still no evidence that a three- or four-group amine-substituted phenyl ring can be effectively synthesized. This limits the ability to investigate the effect of the number and position of amine-functionalized linkers in a physical laboratory. A good alternative is to use computer simulations to model the theoretical amine-functionalized MOFs and study their physical and electronic properties which can serve as a blueprint for further synthetic studies.

Xylene, with the chemical formula of C_8H_{10}, consists of three major isomers namely *ortho*-xylene (ox), *meta*-xylene (mx), and *para*-xylene (px). The separation of xylene isomers is quite challenging owing to their overlapping physicochemical properties (G. Zhang et al. 2021a). The adsorptive separation of xylene isomers is crucial in various processes and industries for optimizing industrial processes, ensuring product quality, and addressing environmental concerns. However, the adsorptive separation of xylenes using porous material has been shown to be highly effective (Y. Yang, Bai, and Guo 2017a). MOFs with "breathing" behavior such as MIL-53 derivatives have been reported

to possess preferential selectivity for xylene isomers (Finsy et al. 2009a). Nevertheless, the effect of non-polar functional groups with different positions on phenyl ring organic linkers on the selective adsorption of xylene isomers could be further investigated. Although there is a broad number of classical simulation studies on the adsorption and separation of xylene isomers, the adsorption of similar structural isomers over MOFs sites is still a challenge since conventional general-purpose force fields based on Lennard–Jones, and electrostatics do not accurately describe them (Fischer, Gomes, and Jorge 2014a). On the other hand, QM approaches can produce accurate adsorption energies and favorable geometries which are in good agreement with experimental reports (Piccini et al. 2015a) (Fellah 2014a).

Although many organic linkers can be functionalized, there are still some limitations. First, certain functional groups can be chemically influenced by solvothermal conditions (high temperature and pressure) which led to producing unwanted crystal structures (Tanabe and Cohen 2011). Also, functionalization methods are sometimes unable to equally distribute a mixture of functional groups on MOF structures (H. Deng et al. 2010). Moreover, depending on functional groups, they could potentially interact with CUS (McDonald et al. 2012). Therefore, it is best to avoid the functionalization of organic linkers for MOFs that contain a high concentration of CUSs such as HKUST-1(Cu) MOF. A potential alternative is the direct replacement of organic linkers with ones containing heteroatoms. Borazine is a compound that has similar structural geometry as benzene (Bettinger, Kar, and Sánchez-García 2009). Since phenyl ring is commonly used as part of organic linkers, the structural features of borazine make it a compelling replacement. Employing borazine as the organic linker fragment in place of phenyl may reduce problems associated with functionalization and generate higher polarity on MOF's surfaces (Fasano et al. 2021). HKUST-1(Cu) has suitable frameworks to be constructed based on borazine as it is rationally designed with tritopic organic linkers and this allows borazine rings to connect to three sides with boron atoms. Using computational methods, this new hypothetical MOF can be modelled and tested. The gas adsorption ability of the hypothetical, borazine-based HKUST-1(Cu) MOF can be compared with the original using DFT and GCMC methods.

One of the prominent problems encountered when considering MOFs as adsorbents is the fact that they cannot be produced in large quantities and the synthesis is usually costly. A proper method for the synthesis of scalable MOF is required to carefully select suitable solvents, reactants, and pieces of equipment. The revised autocorrelations (RACs) analysis using the machine learning (ML) method has recently been updated and there are more than 90,000 synthesized and 500,000 predicted MOF structures (Moosavi et al. 2020). However, among this large number of existing MOFs, only some types of MOFs could be practically employed in pilot-scale production (Ren et al. 2017a). Recently, Shimizu *et al*. have synthesized a highly scalable zinc-based MOF, CALF-20(Zn) (Calgary Framework 20) (Lin et al. 2021). More than 35% of dried solid CALF-20 was extracted per total amount of solvents used, plus an extraordinary space-time yield (STY) for the precipitation step of 550 kg/m^3 per day. Although CALF-20 can be considered a promising scalable MOF for CO_2 adsorption, its capability for the adsorption of other toxic gases has not yet been established. Adsorption of these gases is important in terms of the environmental and health aspects since are among these are the most toxic gases with a high level of immediately dangerous to life or health (IDLH) status (Barea, Montoro, and Navarro 2014) (Korica et al. 2022). Moreover, a study on

the adsorption of such polar and non-polar gases in CALF-20(Zn) would give us a point of view about the chemical environment of the pore surface. Screening the ability of CALF-20(Zn) for the adsorption of polar and non-polar toxic gases will provide an important understanding of the potential of the MOF to be employed in a vast number of applications. This can be achieved using computational methods such as GCMC and MD simulations. Important properties such as adsorption isotherm, loading capacity and interaction energies of polar and non-polar gases can be compared.

1.5 Objectives

The main goal of this project is to utilize computational methods to tackle several issues related to adsorption in MOFs. Adsorption is the key theme for the four different objectives below. The objectives attempt to make clear the impact of some factors on MOF's adsorption. These factors are related and they play an important role on MOF's adsorption. Based on the following objectives, the first and the second items are the effects of polar and non-polar functional groups on MOF's adsorption, respectively. The third objective is the impact of directly employed heteroatom-substituted organic linkers and the last aim is the effect of the polarity of gas molecules on MOF's adsorption. Therefore, the following objectives will be pursued;

1. To determine the effect of different amine-functionalized IRMOF-74-III(Mg) MOFs towards drug adsorption using density functional theory (DFT) calculations and molecular docking simulations

2. To determine the ability of dimethyl-functionalized-MIL53(Al) MOFs for the separation of xylene isomers using DFT calculations

3. To elucidate the influence of organic linker substitution on the adsorption capacity of HKUST-1(Cu) for greenhouse gases using grand canonical Monte Carlo (GCMC) simulations

4. To evaluate the performance of scalable, CALF-20(Zn) MOF in the adsorption of polar and non-polar gases using GCMC and MD simulations.

The theme of the objectives is adsorption. For each objective, the type of MOF was assigned based on the unique feature of the MOF: i) IRMOF-74-III (Mg) contains unsaturated metal sites, and its organic linkers are able to be easily functionalized; ii) MIL-53 (Al) has a breathing effect and has high chemical stability for industry purposes; iii) HKUST-1 (Cu) has a tritopic linker that is suitable for borazine substituting; and iv) CALF-20 (Zn) is scalable and highly stable for gas adsorption purposes.

The scope of work for this research project is designed to address four main objectives, all centered around the pivotal theme of adsorption in MOFs. The first objective focuses on investigating the impact of different amine-functionalized IRMOF-74-III(Mg) MOFs on non-steroidal anti-inflammatory drugs (NSAIDs), employing a combination of DFT calculations and molecular docking simulations. These drug compounds are frequently

used by numerous researchers, as they are cheap and abundantly available in laboratories. Due to the hydrophobic properties of NSAIDs, they are poorly water-soluble, which can result in erratic absorption and low bioavailability. Hence, encapsulating NSAID drug molecules within porous solid materials such as MOFs is highly recommended to improve drug adsorption and delivery. The second objective aims to assess the ability of dimethyl-functionalized-MIL53(Al) MOFs for the separation adsorption of xylene isomers, utilizing DFT calculations. The primary aims try to explain the ability of polar (amine group) and non-polar (methylene group) functionalized MOFs for the adsorption of drug molecules and xylene isomers, respectively. The third objective delves into elucidating the influence of organic linker substitution on the adsorption capacity of HKUST-1(Cu) for greenhouse gases, employing GCMC simulations. This objective emphasizes enhancing CO_2 adsorption into MOFs by preparing borazine-based organic linkers. Lastly, the fourth objective aims to evaluate the performance of scalable CALF-20(Zn) MOF in the adsorption of both polar and non-polar gases, utilizing a combination of GCMC and MD simulations. In this objective, the polarity of gas molecules is taken into account as a crucial factor that influences MOF adsorption. By systematically addressing these objectives, this research endeavours to contribute valuable insights into the multifaceted aspects of MOFs adsorption, shedding light on the effects of various factors such as functional groups, organic linker substitution, and gas polarity on MOF adsorption behavior. The chosen computational methods, including DFT, docking, GCMC, and MD simulations, are tailored to provide a comprehensive understanding of these phenomena, paving the way for advancements in the application of MOFs in adsorption mechanism.

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