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Experimental, Computational and Technological Demands of Atmospheric Water Harvesting

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ABSTRACT **- Atmospheric water harvesting (AWH) has emerged as a viable technological solution to combat global water scarcity, utilising advanced scientific methods to take moisture from the atmosphere and transform it into drinkable water. This article contains a thorough review of the literature with regard to the experimental, computational, and technological demands of AWH systems, including a detailed analysis of the principal aspects affecting system performance and scalability. First, the review includes the characterisation and optimisation of sorbent materials, such as metal-organic frameworks (MOFs), silica gels, and hydrogels, which are essential for improving water adsorption and desorption efficiency. Secondly, the significance of regulated environmental testing to replicate real-world circumstances, evaluate material resilience, and enhance system design for increased water output is delibrated. Thirdly, the computational demands of AWH is discussed in the context of optimising heat and mass transfer mechanisms via computational fluid dynamics (CFD) simulations and molecular dynamics (MD) modelling, which refine material structures and airflow patterns to improve condensation efficiency. Advanced computational techniques, such as machine learning algorithms, are examined to expedite the discovery of high-performance sorbent materials and the optimization of operational parameters across diverse climatic circumstances. Then, the article investigates the incorporation of renewable energy sources, particularly solar power, into AWH systems, evaluating the trade-offs between energy consumption and water output to create sustainable and economically viable solutions. Furthermore, we examine essential elements of water quality evaluation, guaranteeing that collected water adheres to safety regulations via stringent physicochemical and microbiological assessments. Notwithstanding the considerable progress in AWH technology, obstacles persist regarding long-term durability, economic viability, and extensive implementation. Finally, future research must integrate laboratory testing, computational modelling, and field application to create feasible, scalable, and energy-efficient atmospheric water harvesting methods to deliver sustainable water sources globally for arid and water-scarce regions.**

Keywords: Atmospheric Water Harvesting, Sustainable water sources, Arid regions

1.0 INTRODUCTION

Water scarcity is a growing global issue, affecting billions of individuals and ecosystems across the globe (Shemer et al., 2023). Due to growing population increase, urbanisation, and climate change intensifying water stress, novel solutions are urgently required to ensure sustainable water supply (Das et al., 2024). A promising method is atmospheric water harvesting (AWH), a technology that utilises the extensive store of water vapour in the atmosphere. Although freshwater resources provide around 2.5% of total global water, they remain disproportionately scarce despite covering around 71% of the Earth's surface (J. Wang et al., 2025; M. Wang et al., 2024). AWH provides an innovative solution to mitigate water scarcity by harvesting moisture from the atmosphere, particularly in arid and semi-arid areas where traditional water sources are insufficient or unreliable (El-Sharkawy, Haridy, et al., 2024).

Water stress impacts around fifty percent of the global population (Mekonnen & Hoekstra, 2016). Due to the availability of pure water in the environment, porous and hygroscopic sorbents are being studied for the extraction of water from air. An optimal water-harvesting material must (i) absorb water at a favourable relative humidity (RH), including from arid environments, (ii) demonstrate stepwise moisture absorption characteristics to facilitate the uptake and release of substantial water quantities with minimal changes in temperature or pressure, (iii) exhibit efficient water release to minimise energy expenditure and enhance productivity, (iv) possess hydrothermal stability for prolonged functionality, and (v) be composed of non-toxic, readily available materials produced through environmentally sustainable methods.

The concept of AWH is not new. It is inspired by natural processes like dew gathering and fog harvesting, which have been employed by plants and animals for thousands of years (J. Wang et al., 2025). Nevertheless, contemporary progress in material science, thermodynamics, and fluid mechanics has equipped us with the means to create more efficient and scalable AWH systems. These

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technologies, encompassing passive systems like fog nets and active devices utilising desiccants, refrigeration cycles, or sophisticated sorbent materials, has the capacity to transform water accessibility for communities, industries, and agriculture (Glasser & Jenkins, 2018). Nevertheless, despite these encouraging advancements, substantial deficiencies persist in comprehending and enhancing the experimental, computational, and technological requirements of AWH systems.

From an experimental standpoint, the design of AWH systems necessitates meticulous control and manipulation of microclimatic factors, including temperature, humidity, and airflow (M. Wang et al., 2024). Laboratory studies must replicate varied environmental conditions to assess the performance of materials and technology across varying situations. Furthermore, rigorous experimental techniques are essential to evaluate the durability, energy efficiency, and water yield of these systems, thereby confirming their practical applicability in real-world scenarios (Arroyo-Araujo et al., 2022).

Advanced modelling techniques are essential for predicting the performance of AWH systems across spatial and temporal dimensions. Computational fluid dynamics (CFD) simulations can clarify the interactions among airflows, sorbent materials, and heat transfer mechanisms, facilitating the optimisation of system design (Krzywanski et al., 2024). Molecular dynamics (MD) simulations may investigate the adsorption and desorption processes at the atomic level, facilitating the creation of innovative materials with improved water-capturing abilities. Notwithstanding these advancements, the computational complexity of multiscale modelling and the incorporation of experimental data continue to pose considerable obstacles (Salahshoori et al., 2024).

The implementation of AWH systems necessitates the consideration of various practical factors, such as energy demands, material resilience, economic viability, and ecological sustainability (M. Wang et al., 2024). The creation of scalable and modular systems capable of adapting to various climates and water requirements is essential for wider implementation (Nikkhah et al., 2023). Moreover, incorporating renewable energy sources and circular economy ideas into AWH technologies might improve their sustainability and resilience against global environmental concerns (Nikkhah et al., 2023).

In this context, metal–organic frameworks (MOFs) are advantageous materials due to their ease of design and modification to attain specific properties, which has resulted in their effective application for atmospheric water harvesting (Fathieh et al., 2018; Furukawa et al., 2014; Kim et al., 2017, 2018). The discovery of MOF-303 {[Al(OH)(PZDC)], where PZDC2– is 1H-pyrazole-3,5-dicarboxylate; Figure 1a}, represents a major advancement in meeting the previously described sorbent requirements. (Fathieh et al., 2018). Together with the aligned PZDC2-linkers, the aluminium oxide rod-like secondary building units (SBUs; Figure 1b) give the framework hydrothermal stability and produce pores with alternating hydrophilic and hydrophobic pockets. Single-crystal X-ray diffraction study and ab initio molecular dynamics simulations demonstrated that these pockets are optimally configured for the binding of early water molecules, which initiate the development of the overall water structure (Hanikel et al., 2021).

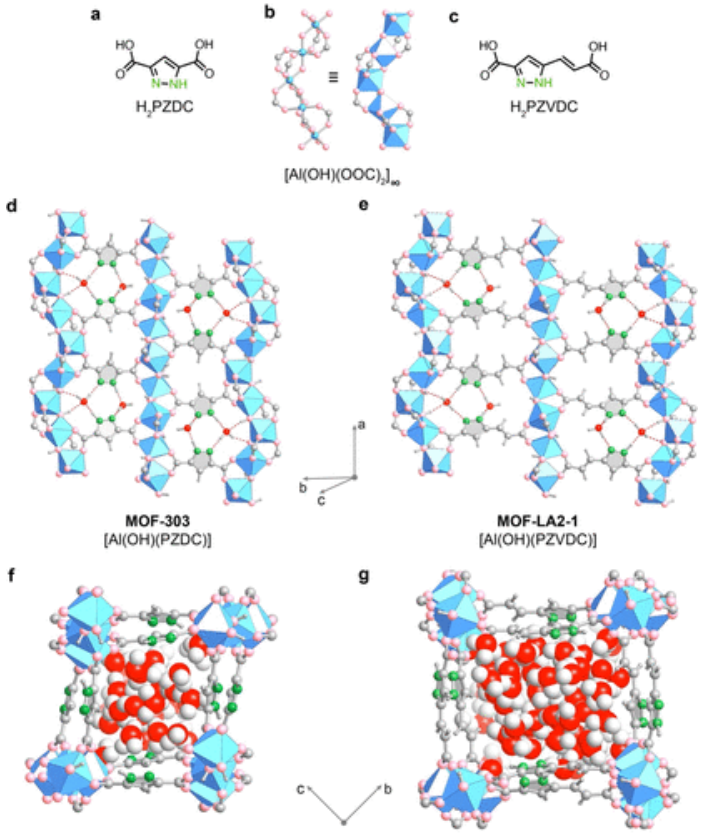

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Figure 1. Comparison of the framework structures and water arrangements in MOF-303 (left) and MOF-LA2-1 (right). (a) The linker 1*H*-pyrazole-3,5-dicarboxylic acid (H_2PZDC) of MOF-303. (b) The aluminum oxide SBU of both MOFs consists of alternating *cis–trans*-corner-shared AlO_6 octahedra. (c) The linker (*E*)-5-(2-carboxyvinyl)-1*H*-pyrazole-3-carboxylic acid (H_2PZVDC) of MOF-LA2-1, where LA2-1 refers to long-arm extension of the linker by two carbon atoms on one side. (d, e) A cut-away view of the pores displaying the alignment of the pyrazole-based linkers such that their hydrophilic N(H) functionalities point toward each other, thus generating an alternating pattern of hydrophilic and hydrophobic pockets. The framework structures and water positions were obtained by a combination of X-ray diffraction analysis and DFT optimization. The hydrophilic pockets serve as strong adsorption sites, which are displayed at a loading of two water molecules per respective asymmetric unit $[Al(OH)(PZDC)]_2$ (d) and $[Al(OH)(PZVDC)]_2$ (e). (f, g) Snapshots of the water structures from Monte Carlo simulations at saturated water loadings of 10 and 18 molecules per asymmetric unit in MOF-303 (f) and MOF-LA2-1 (g), respectively, displayed along the pore channel. Coordinate systems are given for guidance. Al, blue octahedron; C and H, gray; N, green; O in framework, pink; O in H_2O, red (Hanikel et al., 2023)

In the main text, we shall consider the challenge of maintaining the alternating hydrophilic-hydrophobic pocket environment while enhancing the water uptake capacity of the framework, specifically how to augment the pore volume of MOF-303 without sacrificing its advantageous water-uptake properties (Hanikel et al., 2021). The conventional approach to augment the pore volume of aluminium metal-organic frameworks (MOFs) constructed from rodlike secondary building units (SBUs) is linker extension, which entails the use of polycyclic aromatic linkers or the inclusion of extra aromatic rings to the linker (Mishra et al., 2024; T. Wu et al., 2020). Nonetheless, these methods produced hydrophobic, less porous, or large-pore hydrolytically unstable aluminium frameworks (Mishra et al., 2024).

This study aims to examine the experimental, computational, and technological requirements of atmospheric water collection (J. Wang et al., 2025; M. Wang et al., 2024). It seeks to enhance the scientific comprehension of AWH mechanisms, create novel materials and designs, and suggest pragmatic ways to address current limits. This initiative aims to connect basic research with applied engineering to foster a sustainable and equitable future in which access to clean water is a universal right rather than a privilege.

2.0 EXPERIMENTAL DEMANDS

Atmospheric water harvesting (AWH) is a promising solution to the worldwide water scarcity crisis, utilising the planet's abundant atmospheric moisture to provide drinkable water sustainably. Nonetheless, the development of efficient, scalable, and cost-effective AWH systems is fraught with complex experimental problems (Ahrestani et al., 2023; Nikkhah et al., 2023; J. Wang et al., 2025). These issues cover a wide array of scientific and engineering fields, including materials science, thermodynamics, environmental science, and mechanical engineering. Each domain provides distinct experimental requirements that must be carefully addressed to convert AWH from a promising concept into a feasible solution for various contexts and scales (Glasser & Jenkins, 2018). This publication examines the precise experimental requirements necessary to progress AWH technologies, utilising lessons from prior studies and emphasising the essential areas of the current study.

2.1 Ecological Variables and Functional Parameters

The experimental investigation of environmental variables constitutes the foundation of AWH research. The water content in the atmosphere is very changeable, affected by temperature, relative humidity, altitude, and wind patterns. Comprehending these characteristics is essential for customising AWH systems to particular geographic and climatic conditions. Research in arid areas like the Sahara Desert has shown that although relative humidity is generally low, diurnal temperature fluctuations result in elevated absolute humidity during the colder nocturnal hours. Controlled experimental setups have been employed to duplicate these conditions, allowing researchers to refine system designs for enhanced water yield (El-Sharkawy, Haridy, et al., 2024; M. Wang et al., 2024; Zhou et al., 2020).

The significance of wind flow in improving moisture capture efficiency is paramount. Experiments have shown that airflow dynamics considerably influence the rates of water vapour adsorption and desorption in both passive and active systems. Wind tunnel tests have been utilised to replicate natural wind conditions and examine their impact on the performance of different surface shapes. These experiments demonstrate that textured and hydrophobic surfaces promote water collection by generating turbulence that drives moisture towards the sorbent material (Gao et al., 2024; Jarimi et al., 2020). Translating these discoveries into practical

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applications necessitates comprehensive field testing, as real-world conditions can include complexity that are difficult to mimic in laboratory environments (Jarimi et al., 2020). Prior research indicated that the synthesis temperature of unmodified UiO-66 significantly affects its crystallinity and the quantity of structural flaws. Twenty-nine Classical volumetric experiments and the novel quasi-equilibrated temperature-programmed desorption and adsorption (QETPDA) were utilised for the experimental research of water adsorption. Furthermore, density functional theory (DFT) modelling and molecular Monte Carlo simulations were conducted to elucidate the process of water adsorption in UiO-66 derivatives (Jajko et al., 2022; Y. Jiao et al., 2017).

2.2 Optimisation of Sorbent Materials

The advancement and refinement of sorbent materials are fundamental to AWH research. Materials including metal-organic frameworks (MOFs), zeolites, silica gels, and hydrogels have been thoroughly investigated for their capacity to adsorb and desorb water vapour (Bai et al., 2024). Experimental investigations in this field concentrate on assessing critical attributes, such as adsorption capacity, kinetics, thermal stability, and regeneration efficiency (Lu et al., 2023), as depicted in Fig. 2. Also, Fig. 3 also illustrates the mechanisms behind interactions between moisture and sorbents.

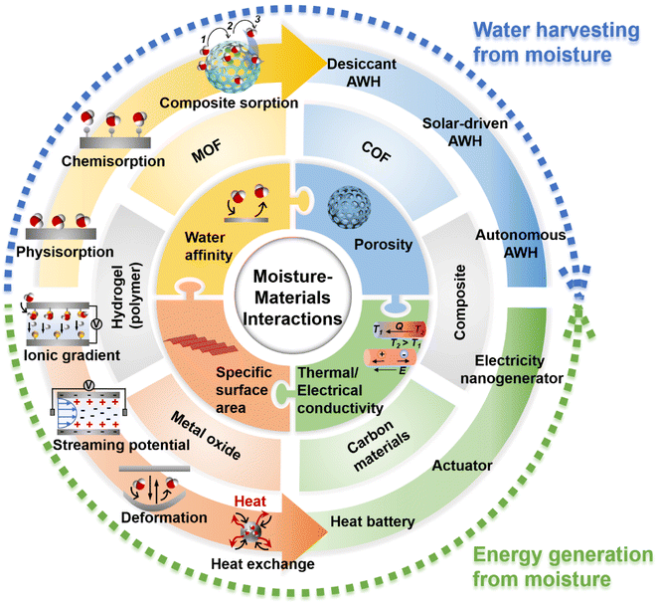

Figure 2. Overview of moisture-enabled water and energy generation technologies (Lu et al., 2023).

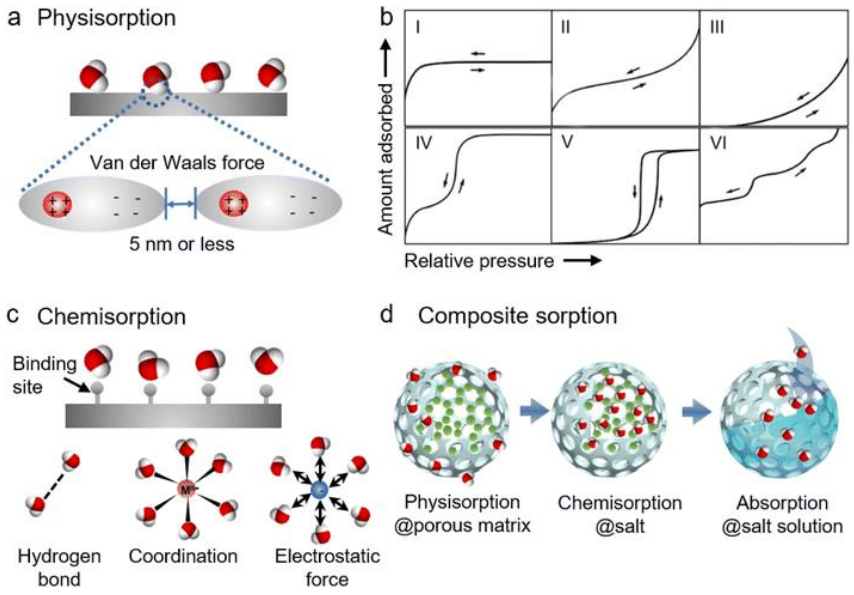

Figure 3. Mechanisms behind interactions between moisture and sorbents: (a) physisorption; (c) chemisorption; and (d) composite sorption. (b) Six types of isotherms describing the physisorption of porous sorbents (Lu et al., 2023)

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MOFs have attracted considerable interest because of their extensive surface area and adjustable pore configurations, enabling selective adsorption of water molecules. Research indicates that the integration of hydrophilic functional groups into metal-organic frameworks (MOFs) improves their ability for water absorption, especially in low-humidity environments (L. Jiao et al., 2019). Nonetheless, these materials frequently encounter issues concerning thermal stability and scalability. Laboratory testing with repeated adsorption-desorption cycles have demonstrated that specific MOFs deteriorate over time, indicating a need for additional research to improve their endurance (Hayat et al., 2024; L. Jiao et al., 2019).

Comparative analyses have underscored the benefits of composite materials that amalgamate the strengths of several sorbents (Bhong et al., 2023). A hybrid material consisting of MOFs and silica gel has demonstrated superior water production and accelerated regeneration times relative to its constituents. Experimental assessments of these composites generally incorporate gravimetric analysis, calorimetry, and spectroscopy to evaluate their performance under diverse environmental circumstances (Bhong et al., 2023; Egbo, 2021). These studies highlight the significance of material innovation in addressing the constraints of current technologies.

2.3 Dynamics of Heat and Mass Transfer

The enhancement of heat and mass transport mechanisms is a crucial experimental requirement in AWH research (X. Li et al., 2024). Effective heat transmission is crucial for facilitating the desorption process, whereas efficient mass transfer guarantees the ongoing transport of water vapour from the atmosphere to the sorbent material (Zhai & Wu, 2021). Advanced diagnostic methodologies, including infrared thermography and computational fluid dynamics (CFD), have been utilised to examine these processes comprehensively (Kesztyüs et al., 2023).

Experiments have shown that the shape and surface area of the sorbent material significantly influence heat and mass transfer rates (Zhai & Wu, 2021). Researchers have evaluated many designs, such as flat plates, packed beds, and honeycomb structures, to identify the ideal design for maximising water yield. CFD models have yielded significant insights into airflow patterns and temperature gradients within these designs, informing the advancement of more efficient systems (Gao et al., 2024).

A significant study utilised 3D-printed prototypes to examine the impact of surface roughness on mass transfer efficiency. The findings indicated that rough surfaces with micro- and nanoscale characteristics generate increased turbulence, enhancing the interaction between water vapour and the sorbent material. These findings have prompted the creation of biomimetic designs that replicate the surface features of real water-harvesting creatures, like desert beetles and cactus (Głowacki et al., 2022; Z. Ma et al., 2024).

2.4 Energy Efficiency and Integration of Renewable Resources

The energy requirements of AWH systems present a considerable problem, especially for active systems dependent on mechanical or thermal energy inputs. Experimental investigations have concentrated on assessing the efficiency of energy-to-water conversion across diverse systems, particularly highlighting the integration of renewable energy sources (Nikkhah et al., 2023).

Solar-powered AWH systems demonstrate significant potential by utilising the plentiful and renewable energy of the sun to facilitate the desorption process. Experiments with photovoltaic-powered desiccant systems have shown water yields reaching 200 millilitres per square metre per day under ideal conditions (Kushwaha et al., 2024). Nonetheless, these systems frequently encounter difficulties concerning energy storage and efficiency degradation during overcast or nocturnal situations. Researchers have investigated the application of phase-change materials (PCMs) for thermal energy storage to provide uninterrupted operation in the absence of direct sunshine (Sadek et al., 2022).

A further area of experimental emphasis is the trade-off between energy use and water yield. For instance, research has contrasted the efficacy of passive systems, which depend exclusively on natural processes like condensation, with active systems that integrate mechanical elements such as fans and pumps. Although active systems typically produce greater water yields, their energy demands frequently constrain their scalability and sustainability. Experiments designed to optimise these trade-offs are essential for creating systems that reconcile performance with environmental and economic factors (Hafez et al., 2023).

Prior research indicates that quantum-chemical calculations of energies and geometries for UiO-66 derivatives were conducted utilising the DMol3 algorithm at the periodic DFT theoretical level (Jajko et al., 2022). The RPBE correlation-exchange functional was employed, and the orbitals were enlarged using the DND basis set with DSPP pseudopotentials (Jajko et al., 2022). Sample Identification: Sample Codes, H2BDC-X Acid Quantities Used, and Synthesis Temperatures Temperature of reaction for H2BDC-

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X/mg (°C) 100.6 120 UiO-66-NH2-170 170 UiO-66-NH2-220 220 H2BDC-NH2 116, 120, UiO-66-NO2-170, 170, UiO-66-NO2-220, 220, UiO-66-Br-120, H2BDC-Br 135 120, UiO-66-Br-170, 170, UiO-66-Br-220, 220(Jajko et al., 2022)

2.5 Water Quality and Long-Term Resilience

Ensuring the safety and reliability of gathered water is a crucial experimental requirement in AWH research. Laboratory analyses have been performed to evaluate the physicochemical and microbiological characteristics of water generated by different systems. These assessments generally utilise spectroscopic and chromatographic methodologies to identify possible pollutants, including heavy metals, organic chemicals, and microbial infections (Essamlali et al., 2024; Narayana et al., 2024).

A study analysed the water quality of samples obtained from a silica gel-based AWH system used in a coastal area. The findings indicated minimal quantities of salts and organic substances, presumably derived from the surrounding atmosphere (Moeinzadeh et al., 2024). Researchers have investigated the incorporation of supplementary filtration and purification stages, including activated carbon filters and UV disinfection units, into the overall system design to mitigate these difficulties (Piai et al., 2022).

Long-term durability studies are crucial, as AWH systems frequently encounter severe environmental conditions that may impair their performance over time (Harle, 2024). Accelerated ageing studies have been performed to assess the impact of elements such as UV radiation, thermal cycling, and mechanical stress on sorbent materials and system components. These experiments yield essential data for enhancing the durability and dependability of AWH technologies, hence ensuring their feasibility for prolonged deployment (Cao et al., 2022; Frigione & Rodríguez-Prieto, 2021).

2.6 Prototype Advancement and Field Evaluations

The shift from laboratory-scale experiments to full-scale prototypes is a pivotal stage in advancing AWH technology. Field trials are crucial for assessing the efficacy of these prototypes in real-world scenarios, offering insights into their scalability, mobility, and user acceptance (Lüdtke et al., 2017).

A significant field trial was implementing a solar-powered MOF-based atmospheric water harvesting system in a remote community with restricted access to potable water (see Fig. 4). The system was engineered for autonomous operation, utilising solar energy to replenish the sorbent material and provide drinkable water to the population. During six months, the system generated an average of 1.5 litres of water daily, underscoring its viability as a sustainable water solution. The trial exposed issues concerning maintenance and user training, highlighting the necessity of incorporating social and logistical factors into system design (J. Wang et al., 2025; Q. Wu et al., 2021).

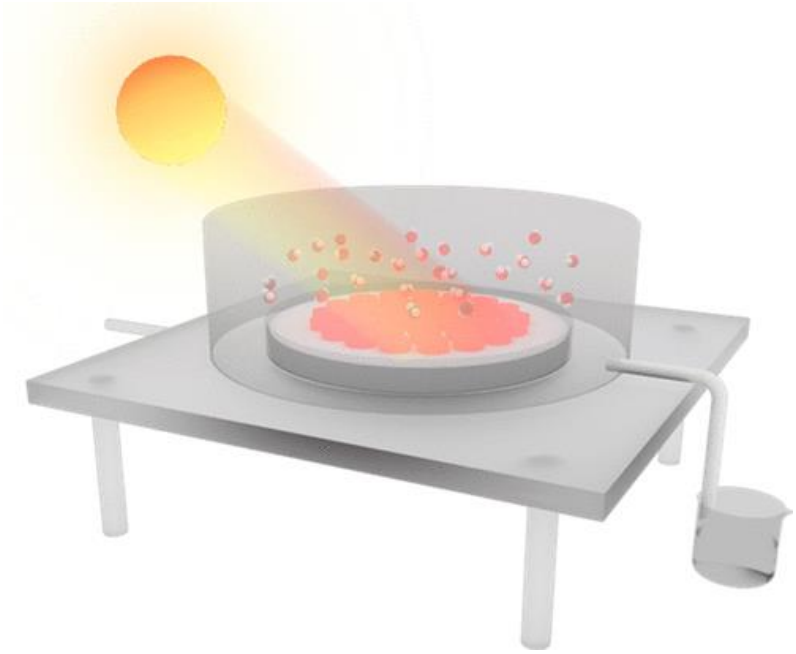

Figure 4. Digital photograph of the assembled SAWH device (Q. Wu et al., 2021)

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3.0 COMPUTATIONAL DEMANDS

The development of materials that can effectively capture and release water vapour necessitates a comprehensive understanding of the molecular and atomic interactions between water molecules and the relevant material surfaces (Gao et al., 2024). Computational simulations are essential for optimising these materials for practical applications. These simulations facilitate the prediction of material behaviour under varying situations and allow for the invention of novel materials with improved features specifically suited for AWH. In this context, computational techniques like Molecular Dynamics (MD), Monte Carlo (MC) simulations, and especially Density Functional Theory (DFT) are critically significant (Krzywanski et al., 2024; Q. Ma et al., 2025). By analysing the benefits and obstacles of various computational techniques, we seek to comprehend how computational modelling facilitates the advancement of next-generation AWH materials (M. Wang et al., 2024).

We now present serially in subsequent sections the three predominant methodologies in AWH research: Molecular Dynamics (MD) simulations, Monte Carlo (MC) simulations, and Density Functional Theory (DFT) (Oukhrib et al., 2021; Paquet & Viktor, 2015). Each solution serves distinct purposes and presents unique advantages and computational obstacles.

3.1 Molecular Dynamics Simulations

Molecular Dynamics (MD) simulations are an effective method for examining the temporal behaviour of molecules. In AWH research, molecular dynamics simulations are employed to explore the movement and interactions of water molecules within porous materials or hydrophilic surfaces. The principal benefit of MD simulations is their capacity to replicate the physical movements of atoms and molecules over time, offering insights into dynamic processes such as adsorption, desorption, and diffusion of water molecules inside the material (Hollingsworth & Dror, 2018; Oukhrib et al., 2021).

MD simulations are commonly employed to investigate the thermodynamic features of materials, including adsorption isotherms, which delineate the quantity of water adsorbed under varying relative humidity conditions. Moreover, molecular dynamics (MD) can assist in examining the influence of environmental variables, including temperature and pressure, on the material's performance regarding water absorption (Filipe & Loura, 2022; Hollingsworth & Dror, 2018). Nonetheless, these simulations are computationally intensive as they necessitate a comprehensive depiction of atomic interactions throughout prolonged timeframes (Khatouri et al., 2022).

The computing requirements in molecular dynamics simulations stem from the necessity to simulate interactions over extended durations, particularly for materials with intricate structures. For example, modelling a singular adsorption event in a material characterised by a substantial surface area or complex pore architecture may necessitate the simulation of thousands of atoms across nanoseconds or even microseconds. As the time steps rise, the computational burden escalates, necessitating access to high-performance computer resources to obtain significant results (Mo et al., 2024)

MD simulations can address many enquiries (Figure 5). This survey highlights prevalent methods, focussing on how simulations often enhance experimental research in molecular biology. The fundamental and intuitive use of simulation is to evaluate the mobility or flexibility of different regions within a biomolecule. Experimental structural determination techniques, including X-ray crystallography and cryo-electron microscopy, typically produce an average structure. By analysing a simulation of this structure, one may measure the movement of different areas of the molecule at equilibrium and identify the types of structural variations they experience. These simulations help elucidate the dynamic behaviour of water molecules and salt ions, which are frequently essential for protein function and ligand binding (Hollingsworth & Dror, 2018; J. Li et al., 2013).

Simulation can be employed to evaluate the precision of a modelled structure. A crystal structure may exhibit artefacts due to crystal lattice packing or, in the case of a membrane protein, due to the lack of a lipid bilayer. Such artefacts can frequently be rectified by initiating a simulation from the crystal structure within a suitably solvated environment, permitting the structure to relax into a more favourable conformation, if available (Burg et al., 2015). A comparable methodology is frequently employed to evaluate the modelled binding conformations of ligands; a pose that demonstrates stability during simulation is more likely to be accurate than one that exhibits instability (Clark et al., 2016). These efforts have demonstrated efficacy in ascertaining ligand orientations in cryo-EM structures exhibiting confusing ligand density (Koehl et al., 2018). MD simulations can be beneficial in enhancing protein homology models; nevertheless, numerous endeavours in this regard have proven unsuccessful (Mirjalili & Feig, 2013).

Conversely, MD simulations are extensively employed to construct or enhance structural models derived from experimental structural biology data. X-ray crystal structures are often revised using a molecular dynamics-based simulated annealing technique that aligns the model with experimental data while preserving a physically plausible structure (Hollingsworth & Dror, 2018). This method has demonstrated the ability to surpass model inaccuracies that least-squares regression fails to address. An MD-based technique is frequently employed to construct atomic-level molecular models from low-resolution cryo-EM density maps, especially

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when high-resolution structures of individual components of a complex are known individually (Zhao et al., 2013). MD simulations have been employed to retrieve ensembles of conformations, rather than a singular structure, from NMR data (Lindorff-Larsen et al., 2005). In each instance, the molecular mechanics force field is augmented with terms reliant on experimental data, yielding a reduced energy for structures (or structural ensembles) that align more closely with the experimental data.

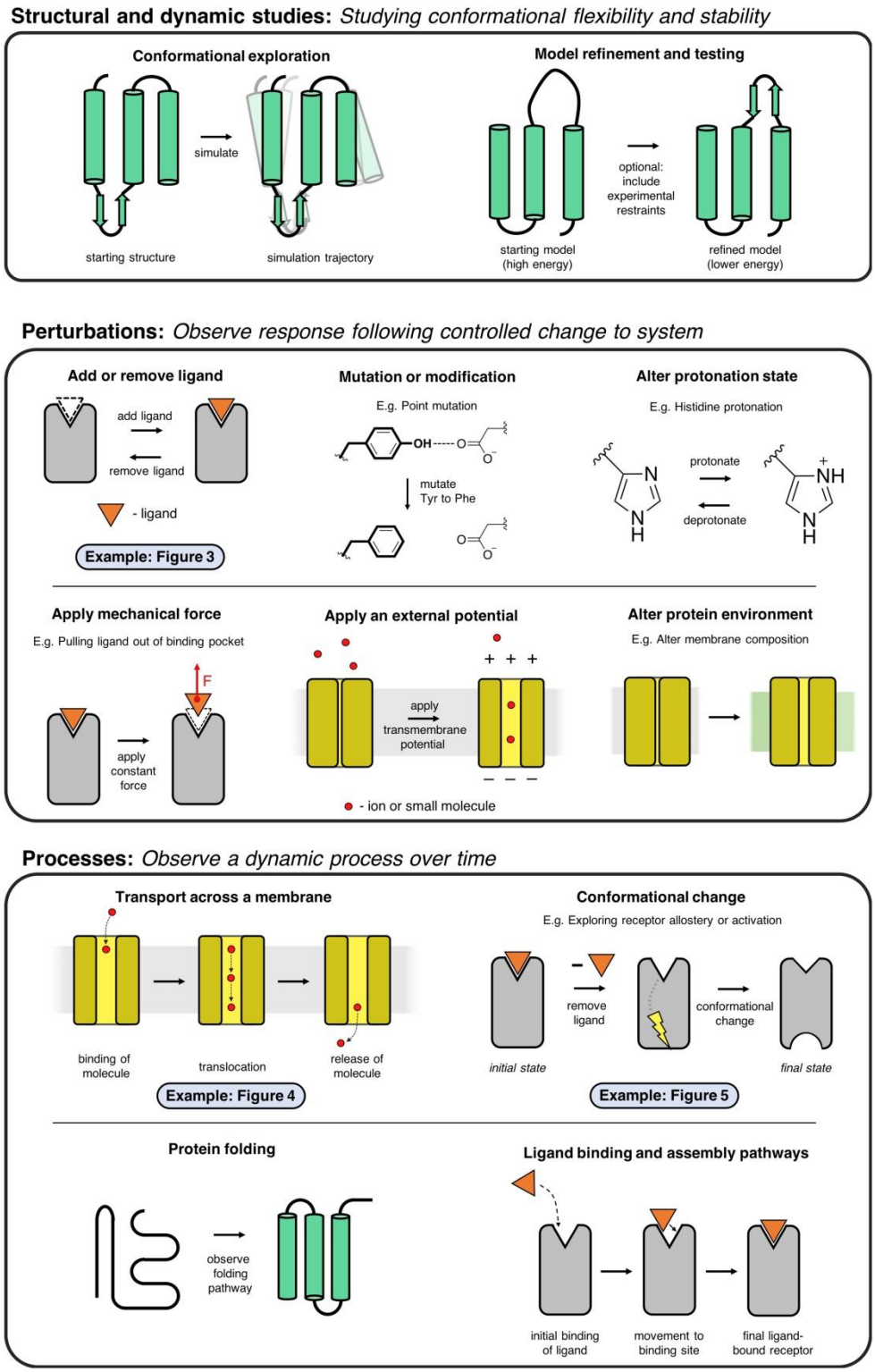

Figure 5. Applications of Molecular Dynamics Simulations (Hollingsworth & Dror, 2018).

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3.2 Monte Carlo Simulations

The phrase "Monte Carlo" originated in the mid-20th century, inspired by the renowned Monte Carlo casino in Monaco, where chance and probability govern results. Currently, Monte Carlo methods are employed across diverse fields, including physics, chemistry, finance, engineering, and environmental research (Harrison et al., 2010; Walter & Barkema, 2015).

Monte Carlo (MC) simulations are a prevalent computational method employed in AWH research, especially in the examination of the equilibrium characteristics of materials. In contrast to molecular dynamics (MD), which emphasises the temporal progression of the system, Monte Carlo (MC) simulations rely on statistical sampling techniques (Harrison et al., 2010). In Monte Carlo simulations, random arrangements of atoms and molecules are produced to determine thermodynamic properties, including adsorption isotherms, pore size distribution, and surface coverage of adsorbed water molecules (Mo et al., 2024).

Monte Carlo simulations are frequently employed to investigate the adsorption characteristics of water molecules in materials like Metal-Organic Frameworks (MOFs), porous hydrogels, and other extremely porous substances. They are especially valuable in assessing how the material's surface area and pore architecture affect the overall efficacy of water adsorption (Chheda et al., 2023).

Although Monte Carlo simulations can be computationally intensive, particularly for systems with numerous particles or intricate pore architectures, they are frequently less time-consuming than molecular dynamics simulations, as they do not necessitate modelling the complete temporal development of the system (Khatouri et al., 2022).

Nonetheless, Monte Carlo simulations necessitate substantial processing resources, especially when addressing disordered materials or extensive systems. Furthermore, the precision of Monte Carlo simulations may be constrained by the selection of sampling technique and the dimensions of the system under simulation (Harrison et al., 2010). These insights are essential for the development of effective materials and systems that can extract potable water from the environment, particularly in arid locations (Chheda et al., 2023). Prior research in the domain of AWH has employed Monte Carlo approaches to elucidate the molecular-level interactions that regulate water harvesting (Chheda et al., 2023; M. Wang et al., 2024). Simulations have been performed to assess the efficacy of metal-organic frameworks (MOFs) and other porous materials in sequestering atmospheric water. This research has illustrated the efficacy of Monte Carlo simulation in forecasting adsorption behaviour, enhancing material qualities, and augmenting the efficiency of water-harvesting technology (Q. Ma et al., 2025).

The concept of employing randomisation definitively was groundbreaking. Its origins can be attributed to the eighteenth century, specifically to Georges Louis LeClerc, Comte de Buffon (1707-1788), a prominent French scientist. He employed stochastic techniques in several experiments, most notably "Buffon's needle," a method using repeated needle throws onto a marked surface to approximate π (Figure 6). LeClerc demonstrated that with a needle equal in length to the distance between the lines, the probability of the needle intersecting a line is $2/\pi$. He evaluated this by hurling baguettes over his shoulder onto a tiled floor. Some regard LeClerc's experiment as the inaugural example of Monte Carlo simulation.

This paper offers a comprehensive examination of Monte Carlo simulation, emphasising its theoretical basis, implementation methods, and applications in AWH research. Particular emphasis is placed on the computing difficulties inherent in these simulations, with methodologies for enhancing their efficiency and precision. By incorporating case studies and practical examples, we seek to offer a thorough comprehension of Monte Carlo simulation and its capacity to enhance the domain of AWH.

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Figure 6. Buffon's Needle: after N tosses, the estimate for pi is (2N/X), where X is the number of times the needle intersects a line (Harrison et al., 2010)

3.2.1 Chronological Evolution of Monte Carlo Simulation

The origins of Monte Carlo simulation date to the early 20th century, with its formal development taking place in the 1940s. Pioneers of probability theory, like Pierre-Simon Laplace and Andrey Kolmogorov, established the foundation for comprehending stochastic processes and random sampling (Harrison et al., 2010). The emergence of sophisticated computing during World War II catalysed the formalisation of Monte Carlo methods. The Monte Carlo simulation became prominent during the Manhattan Project, where it was utilised to model neutron diffusion in nuclear reactors. Stanislaw Ulam, John von Neumann, and Nicholas Metropolis were pivotal in establishing the computing framework for Monte Carlo methods (Archer, 2021; Harrison et al., 2010). Their research illustrated the efficacy of random sampling methods in addressing apparently insurmountable mathematical challenges (Archer, 2021). The adaptability of these methods was promptly acknowledged, resulting in their implementation across various domains like statistical mechanics, finance, and optimisation. Over the decades, Monte Carlo simulation has transformed into a multifaceted computational instrument, bolstered by enhancements in processing capacity and algorithmic innovation. Currently, it is extensively utilised across various disciplines, particularly in material science, where it is crucial for examining adsorption processes and enhancing the efficacy of AWH technologies (Song & Kawai, 2023). A work by Chheda et al. employed Monte Carlo simulations to examine the adsorption characteristics of MOFs for water capture, underscoring the method's capacity to yield comprehensive insights into molecular interactions (Chheda et al., 2023).

3.2.2 Essential Tenets of Monte Carlo Simulation

The Monte Carlo simulation relies on the notion of statistical sampling. The method fundamentally entails obtaining random samples from a probability distribution and employing these samples to estimate numerical outcomes. The precision of the simulation is contingent upon the quantity of samples produced, as more sample sizes diminish statistical error and enhance convergence (Harrison et al., 2010).

1. Mathematical Framework

Let X be a random variable with a specified cumulative distribution function (cdf). The objective of a Monte Carlo simulation is to approximate the expected value of a function, defined as (Zio, 2013):

$$P(X \leq x) = F_X(x);\ F_X(-\infty) = 0;\ F_X(\infty) = 1 \qquad (1)$$

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In the following, if the rv X obeys a cdf we shall write $X \sim F_X(x)$. From the definition, it follows that $F_X(x)$ is a non-decreasing function and we further assume that it is continuous and differentiable at will. The corresponding probability density function (pdf) is then

$$f_X(x) = \frac{\mathrm{d}F_X(x)}{\mathrm{d}x};\ f_X(x) \geq 0;\ \int_{-\infty}^{\infty} f_X(x)\mathrm{d}x = 1 \qquad (2)$$

We now aim at sampling numbers from the cdf $F_X(x)$ A sequence of $N \gg 1$ values $\{X\} \equiv \{x_1, x_2, \ldots, x_N\}$ sampled from $F_X(x)$ must be such that the number n of sampled points falling within an interval $\Delta x \ll X_{\max} - X_{\min}$ (where $X_{\min}$ and $X_{\max}$ are the minimum and maximum values in $\{X\}$) is

$$\frac{n}{N} \simeq \int_{\Delta x} f_X(x)\mathrm{d}x \qquad (3)$$

In a Monte Carlo simulation, this integral is estimated by producing separate random samples and calculating the average.

The precision of this approximation enhances as, in accordance with the rule of large numbers. This notion underpins Monte Carlo methods and facilitates their application to various problems, including integral estimation and the simulation of intricate physical systems (Zio, 2013).

2. Fundamental Concepts

Numerous fundamental notions support the execution and efficacy of Monte Carlo simulations (Harrison et al., 2010):

- Random Sampling: The creation of random samples from a designated probability distribution is fundamental to Monte Carlo methods. Diverse methodologies, including inverse transform sampling and rejection sampling, are employed to accomplish this.
- Tabulation: The procedure of documenting and averaging simulation outcomes is crucial for determining requisite amounts. Counting guarantees that all samples contribute uniformly to the ultimate outcome.
- Variance Reduction: Methods include importance sampling, stratified sampling, and control variates are employed to diminish the statistical error of the simulation and enhance efficiency.
- Convergence Analysis: Observing the convergence of simulation outcomes is essential for guaranteeing precision and dependability. Metrics like confidence intervals and standard error are frequently employed to evaluate convergence.

For example, a work by Icardi et al. utilised Monte Carlo simulations to optimise the pore size distribution of MOFs for AWH applications. The researchers achieved remarkable accuracy at a realistic processing cost by employing modern variance reduction techniques (Icardi et al., 2016).

3.2.3 Techniques of Monte Carlo Simulation

Monte Carlo simulation comprises various methodologies, each designed for particular applications. Within the framework of AWH, these methodologies are especially effective for simulating water adsorption, desorption, and transport phenomena. Herein, we examine several prevalent Monte Carlo approaches employed in scientific research (Pedroni et al., 2017).

- Direct Sampling

Direct sampling entails producing random samples directly from the relevant probability distribution. This approach is direct and effective for uncomplicated distributions, although it becomes problematic for intricate or high-dimensional distributions (L. Wang & Lee, 2014).

- Significance of Importance Sampling

Importance sampling is a variance reduction method that enhances the efficacy of Monte Carlo simulations. Samples are obtained from a proposal distribution that approximates the target distribution, rather than sampling directly from the target distribution itself. The findings are subsequently adjusted to reflect the disparity between the two distributions (Kawai, 2017).

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- Metropolis-Hastings Algorithm

The Metropolis-Hastings algorithm is a prevalent Markov Chain Monte Carlo (MCMC) technique for sampling from intricate probability distributions. This method produces a series of samples by sequentially proposing new states and accepting or rejecting them according to a probabilistic criterion. The Metropolis-Hastings algorithm is especially advantageous for examining adsorption processes in AWH materials (Chib & Greenberg, 1995; Teixeira et al., 2020).

- Gibbs Sampling

Gibbs sampling is an MCMC technique specifically formulated for sampling from multivariate distributions. In each iteration, the algorithm updates a single variable, contingent upon the current values of the remaining variables. Gibbs sampling is frequently employed in statistical modelling and Bayesian inference (Trumbo & Suess, 2018). A work by Abbas et al. employed Gibbs sampling to predict the multivariate adsorption characteristics of water molecules on mixed-ligand MOFs. The findings provide significant insights into the synergistic impacts of several functional groups on water absorption (M. K. Abbas et al., 2024).

3.2.4 Sampling from Probability Distributions

Sampling from probability distributions is a crucial component of Monte Carlo simulation. The selection of a sampling method is contingent upon the distribution's features and the available computational resources.

- Inverse Transform Sampling

Inverse transform sampling is a technique for producing random samples from a cumulative distribution function (CDF). This method is straightforward and efficient for univariate distributions with a mathematically manageable cumulative distribution function (An et al., 2022).

We briefly recap the inverse transform sampling method with one and two variables. In one dimension (1D), let $f(x)$ be a PDF defined on the interval $[a, b]$. Its CDF $F_X(x)$ is a strictly increasing function. To generate N samples $x_1, x_2, \cdots, x_N$ that are distributed according to $f(x)$, we invert the corresponding CDF, that is (An et al., 2022),

$$x_j = F_X^{-1}(u_j)\ (j = 1,2,\cdots,N) \quad (4)$$

where u_j is uniform on [0,1]. This is inverse transform sampling. In practice, we find x_j by finding the root of $F_X(x_j) = u_j$, because the inverse transform F_X^{-1} often cannot be easily obtained. Thus, generating N samples requires solving N root-finding problems.

In two dimensions (2D), let $f(x, y)$ be a joint PDF defined on the rectangular domain $[a, b] \times [c, \mathrm{d}]$. This joint distribution may be written as

$$f(x, y) = f_Y(y) \cdot f_{X|Y}(x \mid y) \quad (5)$$

where f_Y is the marginal distribution in the y direction, and $f_{X|Y}$ is the conditional distribution in the x direction for a given value of y. We do not require that $f(x, y)$ be approximated by a low-rank function as in Ref. Olver & Townsend, 2013, because this approximation is not always valid in our applications. Let F_Y and $F_{X|Y}$ be the CDFs of f_Y and $f_{X|Y}$, respectively. First, N_y samples $y_1, y_2, \cdots, y_{N_y}$ are generated by solving the root-finding problem

$$F_Y(y_k) = u_k,\ (k = 1,2,\cdots,N_y) \quad (6)$$

where u_k is uniform on [0,1]. Second, for each y_k in Equation 3, N_x samples $x_{1k}, x_{2k}, \cdots, x_{N_x k}$ are generated by finding the root for

$$F_{X|Y}(x_{jk} \mid y_k) = u_j,\ (j = 1,2,\cdots,N_x), \quad (7)$$

where u_k is uniform on [0,1]. Thus, sampling of a joint 2D PDF is reduced to sampling of two 1D PDFs. As indicated by Equations (3) and (4), generation of $N_x \cdot N_y$ samples requires solving $(N_x + 1) \cdot N_y$ root-finding problems. In the special case of the separable

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distribution function (i.e., $(x, y) = f_y(y) \cdot f_x(x)$), only $N_x + N_y$ root-finding problems need to be solved to generate N_x. N_y samples.

- Rejection Sampling

Rejection sampling is a versatile method for sampling from intricate distributions. This method involves sampling from a proposal distribution and accepting or rejecting samples based on their likelihood within the target distribution. Although rejection sampling is computationally demanding, it is frequently employed when direct sampling is impractical (Gilks et al., 1995).

Rejection and composirion techniques are used extensively in simulation algorithms for both discrete and continuous distributions. Rejection sampling works by repeatedly simulating random variables from the wrong probability density and then rejecting them with a probability that depends on the ratio of the right density to the wrong density, until an acceptable value is obtained (Gilks et al., 1995).
A very simple example is that of simulating a random variable unifomily distributed on a disk of radius 1 . The rejection method samples a pair (x, y) of independent random variables uniformly distributed on $(-1,1)$ and then rejects the pair unless $x^2 + y^2 < 1$. The rejection probability is either 0 or 1 in this example. This simulates a pair (x, y) uniformly distributed on the unit disk, by the rejection method:

3.2.5 Counting and Decrease of Variability

Effective counting and variance minimisation are essential for achieving precise and dependable outcomes in Monte Carlo simulations. Variance reduction strategies seek to decrease the statistical error of the simulation while maintaining the sample size (Song & Kawai, 2023).

- Significance of Importance Sampling

Importance sampling is a highly effective variance reduction strategy, concentrating computational resources on the most pertinent areas of the probability space. Importance sampling enhances simulation accuracy by allocating greater weights to samples in certain areas (Sandmann, 2007).

- Control Variates

Control variates utilise established correlations among variables to diminish variation. This technique enhances the accuracy of the estimated findings by integrating auxiliary information into the simulation (Yang & Liou, 1996).

- Antithetic Variates

Antithetic variates entail the creation of pairs of negatively linked samples to mitigate random fluctuations. This method is especially effective at diminishing variance in simulations involving symmetric distributions (Cheng, 1984).

3.2.6 Utilisation of Monte Carlo Simulation in AWH

Monte Carlo simulation has been widely employed in AWH research to model water adsorption and enhance system performance. We will examine many principal uses of Monte Carlo simulations in this domain (Chheda et al., 2023).

- Modelling Adsorption Isotherms

Monte Carlo simulations are employed to calculate adsorption isotherms, which delineate the correlation between water absorption and relative humidity. Researchers can assess the capacity and efficiency of AWH materials by simulating the adsorption of water molecules on material surfaces (Afify & Sweatman, 2024).

- Enhancing Material Design

Monte Carlo simulations elucidate the impact of material parameters, including pore size and surface functioning, on water adsorption. These insights are essential for the development of materials with improved performance (Chheda et al., 2023).

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- Forecasting System Performance

Monte Carlo simulations are utilised to forecast the performance of AWH systems under diverse environmental situations. By integrating variables such as temperature, pressure, and humidity, these simulations allow researchers to enhance system designs for practical applications (Pedroni et al., 2017).

3.2.7 Computational Requirements and Obstacles

Monte Carlo simulations, albeit potent, are computationally demanding, especially for intricate systems with high-dimensional probability fields. The computing requirements of Monte Carlo simulations in AWH research emerge from the necessity to model huge systems, conduct thorough sampling, and attain convergence (Harrison et al., 2010; Pedroni et al., 2017).

- Advanced Computational Performance

To tackle these issues, researchers frequently utilise high-performance computing (HPC) capabilities, which facilitate parallel processing and diminish calculation time. Efficient algorithms and variance reduction methods significantly improve the scalability of Monte Carlo simulations (Menon et al., 2023).

- Harmonising Precision and Efficiency

Achieving a balance between accuracy and efficiency presents a significant problem in Monte Carlo simulations. Augmenting the sample size enhances accuracy but concurrently escalates computational expenses. Advanced methodologies, such importance sampling and stratified sampling, assist in alleviating this trade-off (Rajabi & Ataie-Ashtiani, 2014). A work by Li et al. illustrated the application of HPC resources to conduct Monte Carlo simulations for assessing the adsorption behaviour of MOFs under dynamic environmental circumstances. The research emphasised the significance of parallelisation and algorithmic optimisation in fulfilling computational requirements (Z. Li et al., 2024).

3.3 Density Functional Theory (DFT)

Density Functional Theory (DFT) is a prevalent method for examining the electrical structure of materials and their interactions with molecules, such as water. Densitiy Functional Theory (DFT) is predicated on the notion that a system's energy can be ascertained by electron density instead of the intricate many-body wave function (Kohn et al., 1996). This approximation facilitates a considerable decrease in computational complexity relative to alternative quantum mechanical approaches, including the Hartree-Fock approach (A. Abbas et al., 2024).

Within the framework of AWH, DFT is especially advantageous for examining the interactions between water molecules and material surfaces at the atomic or molecular scale (M. Wang et al., 2024). Densely Functional Theory (DFT) offers significant insights into adsorption energies, binding sites, and electronic structures of materials, essential for comprehending the mechanisms of water capture and release in Atmospheric Water Harvesting (AWH) operations (Nikkhah et al., 2023; Zhou et al., 2020). Moreover, DFT allows researchers to investigate the influence of surface functionalisation, pore dimensions, and material composition on water adsorption, depicted in Fig. 7 (Makkar & Ghosh, 2021).

The computing requirements of DFT emerge from the necessity to precisely simulate extensive systems and elucidate nuanced interactions between water molecules and the material interface (Ju et al., 2024). Due to the intricate structures of AWH materials comprising several atoms, DFT computations can be significantly resource-intensive, especially when investigating various configurations of water adsorption. The dimensions of the modelled system, the selection of functionals, and the required accuracy of the outcomes all influence the computing expense of DFT simulations (El-Sharkawy, Gado, et al., 2024).

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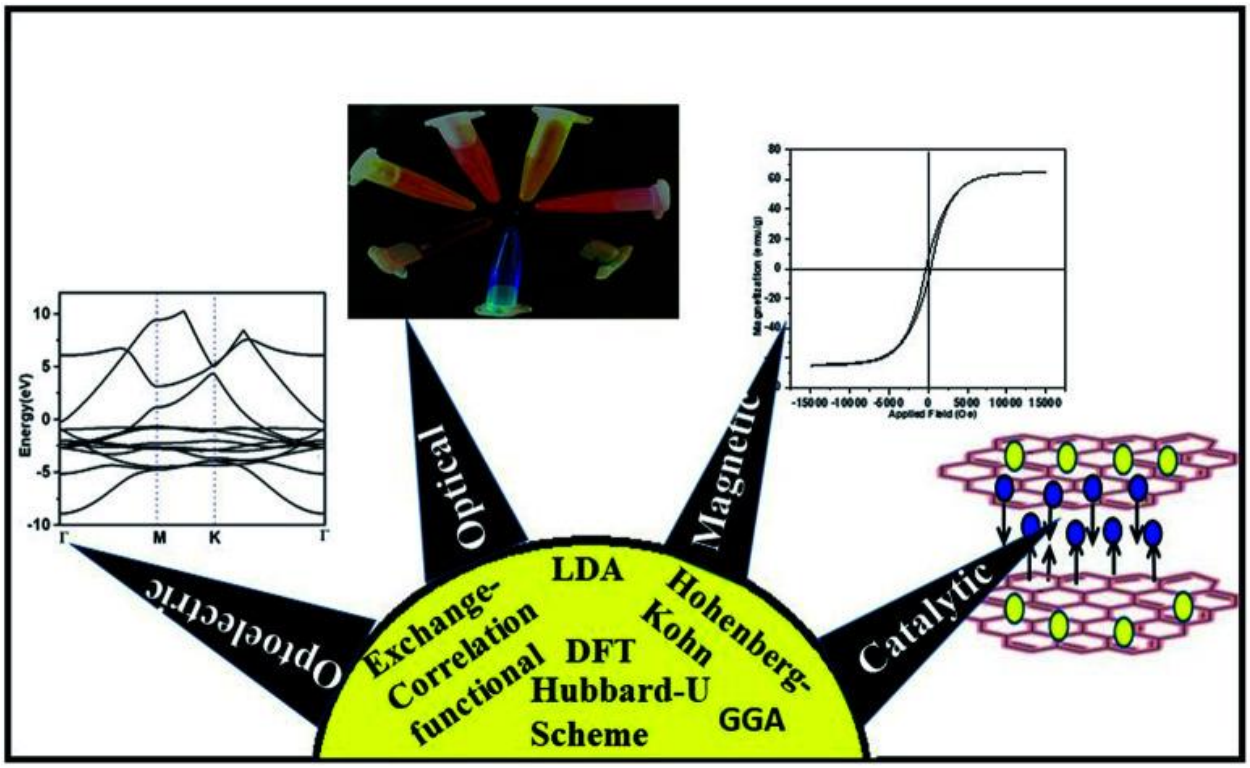

Figure 7. Depiction of unusual properties of nanomaterials through DFT studies (Makkar & Ghosh, 2021).

3.3.1 Computational Requirements of DFT in AWH Investigations

Although DFT is a crucial instrument in the design and optimisation of materials for AWH, it poses considerable computational difficulties, particularly when addressing large, intricate systems. The computing requirements of DFT can be categorised into various critical criteria, including system size, selection of exchange-correlation functional, and the precision needed for the calculations (Ju et al., 2024).

3.3.2 Dimensions of the Systems

A significant problem in employing DFT for AWH investigations is the scale of the systems involved. Numerous materials employed for AWH, including Metal-Organic Frameworks (MOFs), porous hydrogels, and other high-surface-area substances, comprise hundreds or even thousands of atoms (Hu et al., 2023). As the system's size expands, the computational expense escalates correspondingly. The quantity of quantum mechanical calculations necessary to characterise the electronic structure of each atom in a system increases exponentially with the system's size (McCardle, 2023).

Moreover, to precisely depict the adsorption behaviour of water molecules in these materials, researchers frequently need to simulate a substantial quantity of water molecules interacting with the material surface. The quantity of atoms in these systems can rapidly expand to several thousand, leading to a substantial rise in processing time (Salahshoori et al., 2024).

To resolve this difficulty, researchers frequently utilise approximations, such as periodic boundary conditions, to represent extensive systems more effectively. These approximations, although they decrease processing expenses, may also contribute a degree of inaccuracy, particularly when analysing systems characterised by complex interconnections or disorder (Prager et al., 2019; Salahshoori et al., 2024).

3.3.3 Selection of Functional

The selection of exchange-correlation functional in DFT calculations is a crucial element that influences computational requirements. The exchange-correlation functional characterises the many-body interactions among electrons, and choosing a suitable functional is essential for obtaining precise findings (Ryabov et al., 2020). In AWH research, where weak interactions like

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van der Waals forces significantly influence water adsorption, functionals that appropriately characterise these interactions are crucial (Morawietz et al., 2016).
Nevertheless, functionals that employ a more intricate approach to these interactions, such as hybrid functionals or those that include dispersion corrections, are generally more computationally demanding. Conversely, simpler functionals like the Local Density Approximation (LDA) or the Generalised Gradient Approximation (GGA) exhibit more speed but may fail to effectively represent the weak interactions pertinent to water adsorption (Calbo et al., 2015).
Consequently, researchers encounter a trade-off between precision and processing expense when choosing a functional for DFT computations. Although more advanced functionals yield greater accuracy, they necessitate increased processing resources and extended calculation durations (Ledgerwood & Shrout, 2011).

3.3.4 Computational Duration and Convergence

DFT computations frequently necessitate numerous iterations to attain convergence for total energy, electron density, and forces. Attaining convergence is crucial for acquiring dependable data, particularly when analysing intricate systems like water adsorption. The necessity for meticulous convergence testing, especially in the modelling of extensive systems or the examination of minor energy variations, contributes to the total computing expense (Jain et al., 2011; Nakata et al., 2022).
Researchers may conduct several DFT computations for various combinations of water molecules and materials, hence extending the computational duration (Nakata et al., 2022). Furthermore, to precisely represent water adsorption across various situations, several simulations at distinct temperatures, pressures, and relative humidities may be necessary. This requires robust computational resources and the application of efficient techniques to reduce convergence time (Mazur et al., 2024).

3.3.5 Computational Resources

The computer resources necessary for DFT calculations are contingent upon the system's size, the selected functional, and the needed accuracy. In fact, extensive DFT calculations frequently necessitate access to high-performance computing (HPC) clusters or supercomputers, as these systems are capable of managing the substantial volume of computations required for AWH investigations (Ju et al., 2024).
Parallel computing methods are frequently utilised to allocate the computational burden among several processors, hence diminishing the total processing time. Nonetheless, the scalability of DFT computations remains a significant difficulty, particularly when simulating extensive systems with several atoms. Consequently, enhancing the efficiency and scalability of DFT approaches continues to be a pertinent research focus (Schryen, 2020).

3.4 Techniques Employed in Prior Research

Numerous researches have employed DFT to examine the water adsorption characteristics of different materials utilised in AWH, yielding significant insights into the fundamental mechanics. These investigations frequently integrate DFT with additional computational methods, such as MD or MC simulations, to achieve a more thorough comprehension of the material's performance (Jajko et al., 2022).

3.4.1 DFT Investigations on Metal-Organic Frameworks (MOFs)

Metal-Organic Frameworks (MOFs) are a category of porous materials that have been thoroughly investigated for their use in AWH, owing to their substantial surface area and adjustable pore architecture (L. Jiao et al., 2019). A multitude of DFT experiments have been undertaken to investigate the interactions between water molecules and the surfaces of MOFs. Researchers have employed DFT to compute the adsorption energies of water molecules in various MOF structures, ascertain the optimal binding sites, and evaluate the influence of pore size and surface functionality on water absorption (Dasgupta et al., 2021; Jajko et al., 2022).
Makkar & Ghosh (2021) employed DFT calculations to examine the interaction between water molecules and the surface of the MOF-808 material. The findings indicated that adsorption energy was significantly influenced by pore size and surface functional groups, offering critical insights for the development of more effective materials for AWH applications (Makkar & Ghosh, 2021).

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3.4.2 DFT Simulations of Water Clusters

Previous investigations have also employed the simulation of tiny water clusters interacting with material surfaces. These investigations offer essential insights into the hydrogen bonding network of water molecules and the impact of these interactions on adsorption behavior (Sarkisov et al., 2017). Employing DFT to simulate microscopic water clusters enables researchers to get insights into the molecular interactions between water and material surfaces, which is essential for enhancing material qualities for AWH (Dasgupta et al., 2021).

Chen et al. (2019) employed DFT simulations to investigate the interaction of water monomers and clusters with the surfaces of hydrophilic materials. The work elucidated the formation of hydrogen bonds between water molecules and the surface, as well as the influence of these interactions on adsorption energy, offering critical insights for the design of materials with enhanced adsorption capacity (J. Chen et al., 2019).

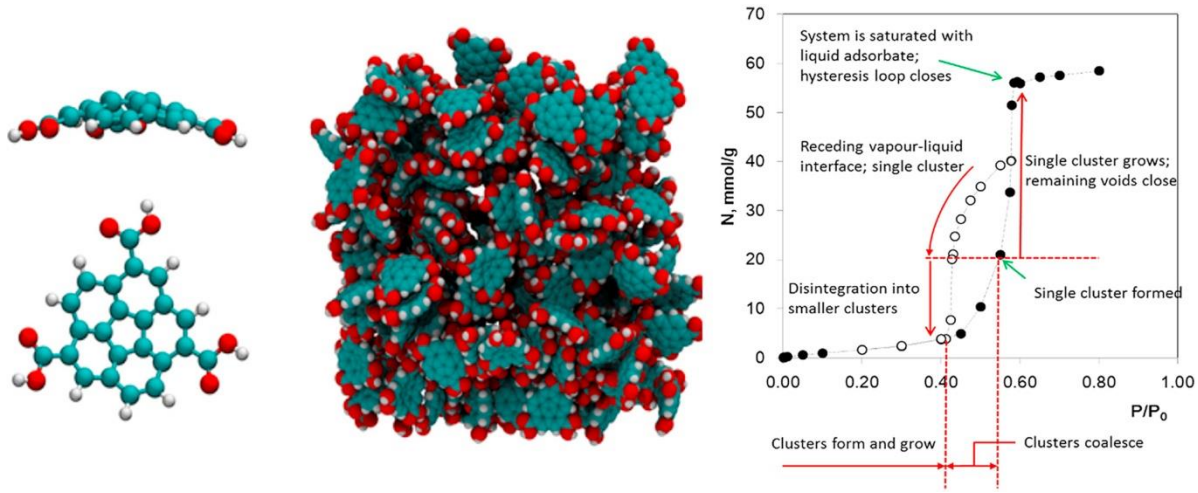

Figure 9. DFT Simulation of water clusters (Sarkisov et al., 2017)

3.4.3 Hybrid Methodologies

In recent years, hybrid methodologies that integrate DFT with alternative techniques, like as MD simulations, have been increasingly prevalent in AWH research. These hybrid techniques allow researchers to model the dynamic behaviour of water molecules in intricate materials while accurately capturing the essential electrical interactions vital for comprehending water adsorption (Rudolph et al., 2024; Schweidtmann et al., 2024). These methods can reduce the computing expense of DFT while maintaining high precision (Nakata et al., 2022).

Hybrid simulations combining DFT and MD have been employed to investigate the transport of water molecules in porous materials. By integrating DFT's precise characterisation of electrical interactions with MD's capacity to simulate molecular dynamics across time, researchers can achieve a more thorough comprehension of adsorption and desorption phenomena (de Haas et al., 2024).

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Box 1: Showcasing the properties of serial hybrid modeling structures

Imagine a system can be manipulated by three factors (inputs), x_1, x_2 and x_3, and the response of the system, which can be measured, is y. If the system is to be modeled by a data-driven model, e.g. a neural network, the model can be posed as:

$$y = f(x_1, x_2, x_3, \mathbf{w}) \quad (1)$$

which implies that x_1, x_2 and x_3, need to be modulated such that the function $f(\cdot)$ (described by the data-driven model) can be inferred and the parameters $\mathbf{w}$ identified (Fig. 1a). Thus, a three-dimensional space needs to be explored to be capable of drawing any conclusions regarding potential interactions between x_1, x_2 and x_3 and/or nonlinearity of the system (within the studied ranges). Considering the system exhibits only main effects and interactions, $2^3 = 8$ experiments are required to decipher the impact of the factors on the system response. Suppose that it is known that the impact of x_3 on y can be described with $x_3/(x_3 + p)$ (with p some parameter), such that the system can be modeled by:

$$y = x_3/(x_3 + p) \cdot f(x_1, x_2, w) \quad (2)$$

The space that needs to be explored in this case comprises only two dimensions (Fig. 1b), namely that of x_1 and x_2. This implies that the number of experiments can be reduced, four experiments are required for the example. In addition, the model will predict reliably for any value of x_3, i.e., the model can extrapolate in x_3 beyond tested values. Regardless of the values in x_3 (except if $x_3 = 0$) the model $f(x_1, x_2, w)$ can be inferred given sufficient variation in x_1 and x_2 (which can exhibit a particular advantage in the case that x_1 or x_2 cannot be controlled). The model $f(x_1, x_2, w)$ will typically be simpler than $f(x_1, x_2, x_3, w)$ which also simplifies the modeling exercise. However, not all of these properties are unique to this specific nonparametric–parametric serial hybrid model sequence. Consider the model shown in Fig. 1c. This structure allows for a reduction in the number of experiments required for the characterization of the system because of the introduced structure (only the impact of g rather than that of x_1 and x_2 needs to be investigated). However, the extrapolation capabilities are different to the model shown in Fig. 1b. This model can be expected to predict well as long as g stays within the prior investigated ranges and hence x_1 and x_2 should only be varied such that g does not exceed this range. In the contrary, the extrapolation limits for x_3 shown in Fig. 1b (and discussed in the example before), are of physical nature in that the model prediction performance will deteriorate when the described mechanism is no longer governing the system behavior.

Figure 10. Properties of serial hybrid modeling structures (Schweidtmann et al., 2024).

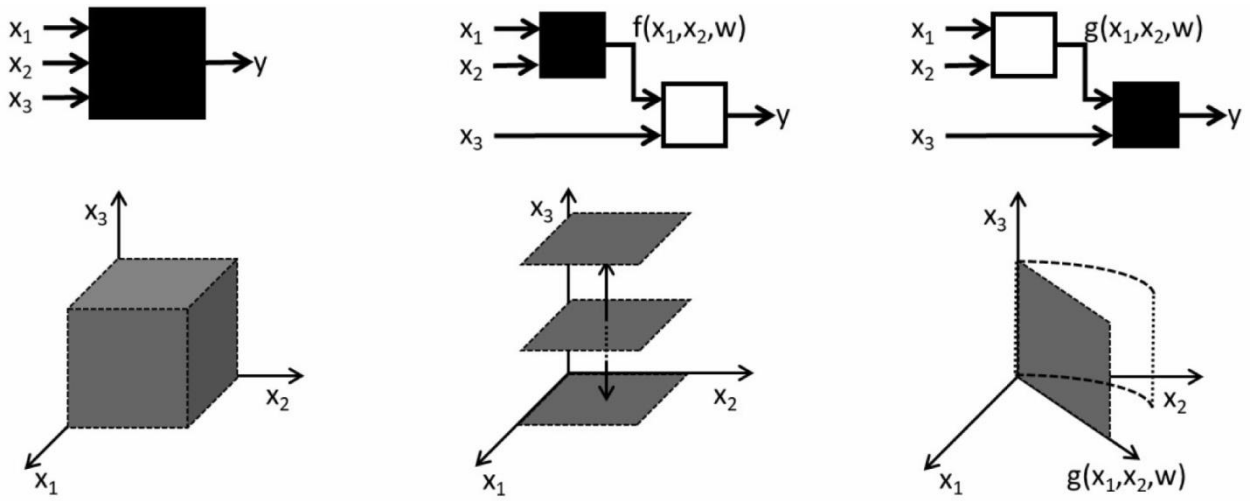

Figure 11. Considering a system with 3 factors (x1 to x3) and response y which only exhibits main effects and interactions, it can be seen that the integration of knowledge has the potential to reduce the experiments. It is considered that f(x1,x2,w) is a function that is given by a machine-learning model, whereas g(x1,x2,w) is a function that is derived from mechanistic knowledge (Schweidtmann et al., 2024).

3.5 Prospective Trajectories and Computational Obstacles

As AWH technology progresses, the computational requirements for simulating water adsorption processes will persistently escalate (M. Wang et al., 2024). Although contemporary techniques like DFT are useful, they possess inherent limits. Anticipated progress in computational methodologies, encompassing the use of machine learning approaches and enhanced algorithms, is projected to alleviate the computational load while preserving precision (Schleder et al., 2019).

Furthermore, the advancement of novel functionals that can more precisely characterise weak interactions, such as van der Waals forces, will be essential for enhancing the accuracy of DFT simulations (Reilly & Tkatchenko, 2015). Furthermore, the utilisation of enhanced high-performance computer resources will empower researchers to model larger systems and investigate more intricate interactions, resulting in the discovery of novel materials and methodologies for AWH (Kelechi et al., 2020).

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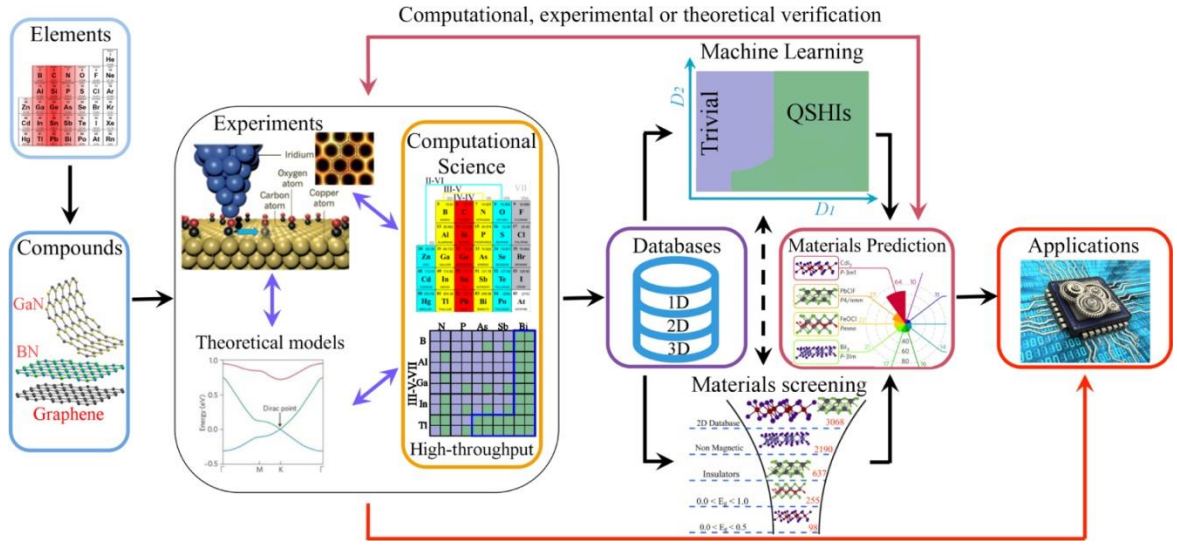

Figure 12. The four science paradigms: empirical, theoretical, computational, and data-driven. Each paradigm both benefits from and contributes to the others (Schleder et al., 2019).

4.0 TECHNOLOGICAL DEMANDS

Water scarcity constitutes a significant global issue, affecting millions who lack access to clean and dependable water sources. This situation is anticipated to escalate owing to population growth, climate change, and heightened industrialization (Shemer et al., 2023). Atmospheric water harvesting (AWH) presents a viable alternative by utilising the extensive store of water vapour in the atmosphere (Nikkhah et al., 2023; J. Wang et al., 2025). With approximately 13,000 trillion liters of water available in the air at any given moment, AWH technologies aim to capture and convert this resource into usable water. Nonetheless, actualising the complete potential of AWH necessitates surmounting considerable technological challenges (Ehtisham et al., 2025). This encompasses the creation of materials with superior water absorption properties, energy-efficient designs, sophisticated computer modelling, and scalable systems appropriate for various environmental situations (Mohammed et al., 2023).

This study examines the methodologies of AWH, emphasises the technological requirements for its implementation, and assesses findings from prior experimental and computational research. This detailed research seeks to elucidate the problems and provide future paths necessary for advancing AWH as a feasible and widespread solution to global water crisis (J. Wang et al., 2025; Zhou et al., 2020).

4.1 Methods of Atmospheric Water Harvesting

Various methods have been devised to extract humidity from the atmosphere. Each approach functions based on a unique basis, exhibiting differing degrees of efficiency, scalability, and technological intricacy. We will analyse the principal methods and the technological prerequisites for their execution (Jarimi et al., 2020).

4.1.1 Condensation-Based Methods

AWH systems that utilise condensation depend on cooling air to its dew point, resulting in the transformation of water vapour into liquid form. This procedure simulates the natural production of dew, wherein water droplets accumulate on surfaces as temperatures decrease overnight (J. Wang et al., 2025). Conventional atmospheric water generators (AWGs) employ refrigeration cycles akin to those in air conditioning systems to produce the cooling effect. Nonetheless, these systems need considerable energy input to function compressors and cooling units (Shafeian et al., 2022). In low-humidity conditions, the energy requirements escalate considerably, rendering traditional AWGs unsuitable for extensive implementation. Recent improvements have investigated alternative cooling techniques, including thermoelectric cooling, desiccant-assisted cooling, and hybrid systems that incorporate solar energy to diminish reliance on power (Komazaki et al., 2025).

A key technological requirement in condensation-based atmospheric water harvesting is enhancing energy efficiency. Researchers are examining new materials with elevated thermal conductivity to improve heat exchange efficiency (J. Wang et al., 2025).

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Furthermore, innovative system designs utilising phase-change materials (PCMs) have been investigated to store and release thermal energy, enhancing condensation rates while minimising energy usage (Morciano et al., 2025).
A further problem is maintaining uninterrupted operation under diverse air conditions. Computational modelling is essential for forecasting dew point variations and enhancing system efficiency correspondingly (Shaier et al., 2025). Machine learning techniques have been utilised to optimise operational parameters by dynamically altering cooling intensity in accordance with real-time meteorological data (M. Wang et al., 2024).

4.1.2 Sorption-Based Methods

AWH systems based on sorption employ specific materials, referred to as sorbents, capable of capturing and releasing water vapour. These materials are generally categorised into two classifications (Ehtisham et al., 2025; J. Wang et al., 2025):

- Absorbents: Substances that chemically interact with water, including hygroscopic salts (e.g., lithium chloride, calcium chloride).
- Adsorbents: Substances that physically capture water molecules on their surfaces, such as silica gel, zeolites, metal-organic frameworks (MOFs), and hydrogels.

Sorption-based atmospheric water harvesting (AWH) systems do not necessitate substantial energy input for chilling, in contrast to condensation-based systems. Rather, it depends on temperature variations to initiate the release of accumulated water (Bai et al., 2024). In passive systems, moisture is released when ambient temperature increases, facilitating water collecting without other energy sources (Bai et al., 2024).
The technological requirement in this domain centres on the creation of high-performance sorbents with improved water absorption capacity and expedited regeneration cycles. Researchers are developing novel metal-organic frameworks (MOFs) with enhanced pore architectures, facilitating increased water retention and reduced desorption temperatures (Naeem et al., 2018). Hydrogels, modelled after biological systems like desert flora, have been designed to demonstrate fast water absorption and release capabilities.
Computational chemistry has been instrumental in the discovery of novel sorbent materials. Molecular simulations allow scientists to anticipate the adsorption characteristics of various substances, facilitating the creation of extremely efficient water-harvesting materials. The experimental validation of these computational models guarantees that actual performance corresponds with theoretical predictions (Kumi et al., 2024).

4.1.3 Fog Harvesting

Fog harvesting is a passive technique for collecting water droplets from misty air utilising mesh structures. This strategy has been effectively employed in coastal and hilly areas where fog frequently occurs. The design of fog nets is essential for optimising water collecting efficiency. Optimised mesh materials, coatings, and surface structures can improve droplet coalescence and reduce water loss from re-evaporation (Qadir et al., 2021).
A primary technological requirement in fog harvesting is the creation of superhydrophilic and superhydrophobic coatings. These specialised coatings facilitate the movement of water droplets towards collection reservoirs while inhibiting clogging and microbiological proliferation. Researchers have drawn inspiration from nature by examining the surface characteristics of beetles and spider silk to create biomimetic fog-harvesting materials (Oktor et al., 2024).
Moreover, computational fluid dynamics (CFD) simulations have been utilised to model airflow patterns and enhance the positioning of fog collection systems. These models enable engineers to devise structures that optimise water capture efficiency and reduce airflow resistance (Caron et al., 2025).

4.2 Technological Demands of Atmospheric Water Harvesting

For AWH systems to achieve practicality and widespread adoption, they must satisfy many technological prerequisites. The subsequent sections address the essential domains requiring progress (El-Sharkawy, Haridy, et al., 2024).

4.2.1 Material Development

The efficacy of AWH technologies is predominantly contingent upon the materials employed for water capture, retention, and release. Essential factors in material growth encompass (J. Wang et al., 2025; M. Wang et al., 2024; Zhou et al., 2020):

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- High Water Absorption Capacity: Materials must effectively absorb or condense water vapour, especially under low-humidity conditions.
- Low-Energy Regeneration: Sorbents must discharge retained water with low thermal input to optimise energy efficiency.
- Durability and Longevity: Materials must endure numerous cycles of absorption and desorption without substantial deterioration.
- Environmental Safety: Preference is given to non-toxic, biodegradable, and eco-friendly materials for sustainable implementation.

Recent advancements in materials science have concentrated on the development of next-generation sorbents. Metal-organic frameworks (MOFs) have garnered interest owing to their adjustable pore architectures and remarkable water adsorption capabilities. Researchers are investigating hybrid materials that integrate the advantages of hydrogels with metal-organic frameworks (MOFs), resulting in composite sorbents with enhanced performance attributes (Felix Sahayaraj et al., 2023; Muthukumaran et al., 2025).

4.2.2 Energy Efficiency and Sustainability

AWH technologies must be designed with energy efficiency in mind. Numerous contemporary systems necessitate external power sources, rendering them unsuitable for off-grid applications. In response, researchers are creating passive atmospheric water harvesting devices that utilise natural temperature fluctuations to facilitate water collection (M. Wang et al., 2024).
Solar-assisted atmospheric water harvesting systems represent a potential methodology. By including photovoltaic panels or solar thermal collectors, these systems can produce the requisite energy for cooling or desorption operations independently of traditional electrical networks (Q. Wu et al., 2021). Progress in thermoelectric materials has facilitated the creation of self-sustaining AWH devices, enhancing energy sustainability (Q. Wu et al., 2021).

4.2.3 Computational Modeling and System Optimization

Computational modelling is crucial for optimising Automated Warehouse Handling systems. Diverse numerical methods are employed to model water adsorption behaviour, heat transfer dynamics, and airflow patterns. These models assist researchers in detecting design deficiencies, forecasting performance across various environmental circumstances, and optimising system configurations (Z. Chen et al., 2025).
Machine learning methods have been used into AWH development to improve forecasting precision. AI-driven solutions can optimise harvesting tactics by analysing historical weather data and altering operational parameters in real time to enhance efficiency (Bojer, 2022).
Moreover, digital twins—virtual representations of physical AWH systems—enable engineers to do virtual trials and evaluate adjustments prior to applying changes to real-world prototypes. This methodology dramatically decreases the time and expenses related to trial-and-error experimentation (Papachristou et al., 2024).

4.2.4 Scalability and Practical Implementation

For AWH to achieve substantial worldwide influence, systems must be both scalable and economically viable. Presently, high-performance materials like MOFs are costly to synthesise and produce on a big scale. Confronting this challenge necessitates innovation in material manufacturing techniques and supply chain operations (Hu et al., 2023; M. Wang et al., 2024).
A vital component of scalability is the incorporation of AWH systems into the current infrastructure. Researchers are investigating methods to integrate water-harvesting materials into building facades, rooftop systems, and agricultural irrigation networks. Integrating AWH technology into urban and rural locations enhances water security across various contexts (J. Wang et al., 2025; M. Wang et al., 2024).

4.2.5 Field Testing and Real-World Applications

Notwithstanding favourable laboratory outcomes, numerous AWH devices remain inadequately evaluated in practical environments. Fluctuations in temperature, humidity, wind patterns, and air quality can affect system performance. Prolonged field investigations are essential to evaluate durability, maintenance needs, and overall efficacy (Chaudhry et al., 2023).

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Pilot initiatives in arid locations are yielding significant insights into practical issues and user requirements. Community involvement and local collaborations are crucial for effective implementation, guaranteeing that AWH solutions correspond with the socioeconomic and cultural circumstances of the targeted regions (Xing & Wang, 2024; Zhang et al., 2023).

5.0 DISCUSSION

The investigation of atmospheric water harvesting (AWH) as a feasible remedy for water scarcity necessitates a comprehensive strategy that combines experimental study, computer modelling, and technological innovations (J. Wang et al., 2025). The previous sections have offered a detailed analysis of these requirements, emphasising the complex interactions among environmental factors, materials science, fluid dynamics, thermodynamic processes, and overall system efficiency. This discourse rigorously investigates the predominant themes arising from these elements, highlighting the interconnections among experimental approaches, computational analyses, and technical advancements in enhancing AWH systems.

Experimental research is fundamental to AWH developments, providing essential insights on material performance, system efficiency, and environmental adaptability. AWH systems depend significantly on optimised sorbent materials, advances in heat and mass transfer, and regulated environmental testing to guarantee consistent water production across various situations (M. Wang et al., 2024). The experimental component of this study emphasised the need of laboratory assessments for characterising sorbent materials, such as metal-organic frameworks (MOFs), silica gels, and hydrogels. These materials demonstrate varying adsorption capacities, kinetics, and regeneration efficiencies, requiring controlled experiments to determine the most successful candidates for large-scale application (Han et al., 2019; Pellenz et al., 2023).

A primary experimental issue in AWH is the replication of authentic climatic conditions in laboratory environments. The fluctuations in humidity, temperature, and airflow across various geographical areas need the implementation of controlled environmental chambers and field testing to substantiate laboratory results. Laboratory trials, although essential for characterising material behaviour, must be supplemented with real-world applications to evaluate durability, energy efficiency, and long-term viability. Moreover, the effects of environmental pollutants, microbial contamination, and material degradation due to extended exposure to ultraviolet (UV) radiation and air contaminants must be examined through stringent testing techniques (Chaudhry et al., 2023).

In addition to material optimisation, experimental study has concentrated on enhancing water collection methods via structural and design alterations. Surface texturing, airflow directionality, and passive cooling methods have been investigated to improve water condensation and collection efficiency. Computational fluid dynamics (CFD) simulations, thoroughly examined in the computational section, are essential in these experimental endeavours by informing design iterations and reducing energy losses. Despite considerable advancements in the experimental field, additional research is required to enhance energy efficiency, bolster long-term system stability, and create economically viable AWH prototypes suitable for deployment in water-scarce areas (Caron et al., 2025).

The computational requirements of AWH involve several modelling techniques that aid in material selection, system design, and operational efficiency. Computational fluid dynamics (CFD), molecular dynamics (MD) simulations, thermodynamic modelling, and machine learning applications have significantly enhanced AWH technology. Utilising these computational methods, researchers may examine airflow dynamics, improved heat and mass transfer processes, and forecast the adsorption-desorption behaviour of sorbent materials across various environmental circumstances (Krzywanski et al., 2024; J. Wang et al., 2025; M. Wang et al., 2024).

CFD models have yielded significant insights into optimising airflow patterns surrounding sorbent materials to enhance water capture. The aerodynamic performance of AWH prototypes, encompassing both passive and active collection systems, has been thoroughly modelled to pinpoint design enhancements that increase water yield while reducing energy consumption (Caron et al., 2025). Nonetheless, the substantial computational expense of CFD simulations persists as a hurdle, necessitating sophisticated meshing approaches, parallel computing, and machine learning-based surrogate models to expedite simulations without sacrificing accuracy (Caron et al., 2025).

Molecular dynamics (MD) simulations have greatly enhanced the optimisation of sorbent materials by offering atomistic insights into the interactions of water molecules with porous structures. The simulations indicate that the strategic positioning of hydrophilic functional groups in metal-organic frameworks (MOFs) can markedly improve water uptake efficiency (Hollingsworth & Dror, 2018). Notwithstanding these developments, molecular dynamics simulations necessitate substantial computational resources, especially when modelling large-scale systems over prolonged durations. Future developments in quantum computing and improved sampling techniques may provide solutions to these computational problems, facilitating more efficient material screening processes.

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Applications of machine learning and artificial intelligence (AI) have arisen as potent instruments for AWH optimisation. Predictive models developed from experimental and simulation data can expedite material discovery, enhance operational parameters, and elevate system performance across diverse environmental circumstances. Neural networks have been utilised to predict water yield based on humidity, temperature variations, and material characteristics, thereby diminishing dependence on expensive and time-intensive physical trials. The amalgamation of AI with physical simulations and empirical testing needs additional investigation, especially in the creation of interpretable models capable of generalising across varied environmental circumstances.

Technological breakthroughs in AWH include not only material and computational enhancements but also system-level integration, energy efficiency factors, and practical implementation issues. Passive AWH systems, dependent on natural condensation and adsorption mechanisms, have shown potential in low-energy applications but frequently have constrained water output. Conversely, active AWH systems utilise energy-demanding processes such as desorption heating, mechanical compression, or refrigeration to improve water recovery rates. It is crucial to balance these trade-offs to create sustainable AWH systems that conform to energy supply and cost limitations (M. Wang et al., 2024; Zhou et al., 2020).

A significant technological achievement in AWH has been the incorporation of renewable energy sources, including solar electricity, into system designs. Solar-assisted desorption has demonstrated efficacy in minimising external energy requirements while sustaining elevated water recovery rates. The exploration of hybrid systems integrating passive and active harvesting techniques has been undertaken to enhance efficiency while minimising energy consumption increases (Zhou et al., 2020). Nonetheless, attaining extensive acceptance of these technologies necessitates additional advancements in energy storage, automation, and adaptive system controls (Lu et al., 2023).

A pivotal factor in the advancement of AWH technology is the quality of the extracted water. To ensure that the collected water complies with safety regulations for human consumption, it is imperative to conduct thorough testing for potential contaminants, such as volatile organic compounds (VOCs), leachates from sorbent materials, and microbiological proliferation (Ehtisham et al., 2025; J. Wang et al., 2025). Computational models, integrated with real-time monitoring devices, have been suggested as solutions for ongoing water quality evaluation, facilitating preventive measures when contamination threats are identified. Future research ought to concentrate on the integration of water treatment technologies, including UV sterilisation and filtration, into AWH systems to guarantee consistent water quality (Essamlali et al., 2024).

The scalability and economic feasibility of AWH technologies are critical difficulties that must be resolved to enable extensive use. Techno-economic analyses have been utilised to evaluate cost determinants, encompassing material synthesis, energy consumption, maintenance needs, and system durability (M. Wang et al., 2024). These evaluations offer critical insights into the trade-offs between performance enhancements and cost ramifications, informing investment decisions and policy frameworks. Field trials and pilot-scale demonstrations are crucial for proving the economic viability of AWH technology and determining strategies for large-scale adoption.

6.0 CONCLUSION

The progression of AWH technology necessitates a multidisciplinary approach, demanding ongoing innovation across experimental, computational, and system-level fields. The experimental prerequisites for atmospheric water harvesting encompass a wide array of scientific and engineering challenges that must be addressed to realise the technology's complete potential. AWH research requires comprehensive experimentation and interdisciplinary collaboration, including the optimisation of sorbent materials, heat transfer methods, water quality assurance, and system resilience. Computational studies are essential for the advancement of AWH devices, providing valuable insights into the interactions between water molecules and materials. Notwithstanding its processing demands, DFT serves as a potent tool for understanding atomic-level interactions. By overcoming current computational challenges and enhancing algorithms and computing resources, the field of AWH is anticipated to make continuous progress in the development of more efficient and sustainable materials for atmospheric water capture. Addressing the technology requirements and constraints identified in this study is crucial for attaining widespread adoption.

Ongoing research and innovation in materials development, energy efficiency, system scalability, and interaction with existing infrastructure will be essential for the advancement of AWH. Through joint initiatives and ongoing investment, AWH technologies can play a crucial role in securing water resources for future generations. Future research should emphasise the incorporation of contemporary technology, such as artificial intelligence and machine learning, to enhance system efficacy and adaptability. The development of hybrid systems that combine AWH with alternative water treatment and storage techniques may offer new opportunities for innovation. By fulfilling these experimental criteria, researchers can promote the widespread adoption of AWH technologies, advancing a more sustainable and water-secure future.

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