

## Article

# Counter-Intuitive Magneto-Water-Wetting Effect to CO<sub>2</sub> Adsorption at Room Temperature Using MgO/Mg(OH)<sub>2</sub> Nanocomposites

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**Abstract:** MgO/Mg(OH)<sub>2</sub>-based materials have been intensively explored for CO<sub>2</sub> adsorption due to their high theoretical but low practical CO<sub>2</sub> capture efficiency. Our previous study on the effect of H<sub>2</sub>O wetting on CO<sub>2</sub> adsorption in MgO/Mg(OH)<sub>2</sub> nanostructures found that the presence of H<sub>2</sub>O molecules significantly increases (decreases) CO<sub>2</sub> adsorption on the MgO (Mg(OH)<sub>2</sub>) surface. Furthermore, the magneto-water-wetting technique is used to improve the CO<sub>2</sub> capture efficiency of various nanofluids by increasing the mass transfer efficiency of nanobeads. However, the influence of magneto-wetting to the CO<sub>2</sub> adsorption at nanobead surfaces remains unknown. The effect of magneto-water-wetting on CO<sub>2</sub> adsorption on MgO/Mg(OH)<sub>2</sub> nanocomposites was investigated experimentally in this study. Contrary to popular belief, magneto-water-wetting does not always increase CO<sub>2</sub> adsorption; in fact, if Mg(OH)<sub>2</sub> dominates in the nanocomposite, it can actually decrease CO<sub>2</sub> adsorption. As a result of our structural research, we hypothesized that the creation of a thin H<sub>2</sub>O layer between nanograins prevents CO<sub>2</sub> from flowing through, hence slowing down CO<sub>2</sub> adsorption during the carbon-hydration aging process. Finally, the magneto-water-wetting technique can be used to control the carbon-hydration process and uncover both novel insights and discoveries of CO<sub>2</sub> capture from air at room temperature to guide the design and development of ferrofluid devices for biomedical and energy applications.

**Keywords:** room temperature; CO<sub>2</sub> adsorption; magneto-wetting; nesquehonite; aging



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## 1. Introduction

At present, renewable energy sources are garnering much attention due to their many advantages, including many environmental benefits [1]. However, in spite of the advantages, the majority of the energy requirements are fulfilled by utilizing fossil fuels. There are many adverse effects associated with anthropogenic activities, especially fossil fuel combustion, which contributes to the emission of carbon dioxide gas at an alarming rate. Compelling evidence supports the fact that the constant emission of CO<sub>2</sub> gas into the atmosphere is the leading cause of global warming. Apart from that, accumulated gas in the atmosphere brings a series of adverse events such as air pollution, extreme weather conditions, etc. Hence, high levels of CO<sub>2</sub> in the atmosphere are an alarming threat to all living beings in the world. Therefore, to mitigate these negative impacts, CO<sub>2</sub> capture, and storage have gained the great interest of many research groups.

Consequently, the use of sorbent materials for carbon capture has received a great deal of attention. These materials include both solid and liquid-based materials. Solid adsorbents have its advantages over liquid adsorbents [2]. The use of solid adsorbents,

such as metal organic frameworks (MOFs) [3–6], metal oxides [7–10], polymer-based sorbents [11–13], zeolites [14,15], etc., is now being heavily investigated. Although they perform well in CO<sub>2</sub> adsorption, they require high temperature and/or pressure gradients to enable efficient sorption capacities. Particularly the use of magnesium hydroxide (Mg(OH)<sub>2</sub>) to produce magnesium oxide (MgO)-based adsorbents is gaining popularity due to a number of reasons, including its ability to capture CO<sub>2</sub> at intermediate temperatures, low cost, availability, and non-toxicity [16,17]. Among the many advantages, Mg(OH)<sub>2</sub> powder has been a widely used raw material in producing MgO for CO<sub>2</sub> capture. Numerous experimental projects have been involved in investigating the production of Mg(OH)<sub>2</sub> powder from the discharged brine from desalination plants [2,18–20], which has the potential to generate more economic and environmental benefits at the commercial scale production of MgO-based CO<sub>2</sub> adsorbents.

Among many attempts to use pure MgO as a CO<sub>2</sub> adsorbent, the capture capacities have been relatively low compared to other adsorbents mainly due to its fewer active sites to capture CO<sub>2</sub> [21,22]. Apart from that, long-term CO<sub>2</sub> fixation with MgO to produce thermodynamically stable magnesium carbonates (MgCO<sub>3</sub>) hinders further adsorption of CO<sub>2</sub> on MgO. Gregg et al. [23] used pure MgO for CO<sub>2</sub> adsorption and were able to obtain 0.4 mmol g<sup>-1</sup>, but since then, many studies have reported improved adsorption rates of pure MgO and MgO-based adsorbents at different conditions. MgO samples prepared by various methods affect the physical properties, which affects their performance in terms of CO<sub>2</sub> capture. Subsequently, to improve the capture performance of MgO, various approaches have been reported [8,24–29].

The effect of an external magnetic field on sorbents for CO<sub>2</sub> adsorption has been studied by many for different types of sorbent materials. The mass transfer enhancement using external magnetic fields has been studied [30–32]. In a study by Samadi et al. [30], a magnetic field was applied on Fe<sub>3</sub>O<sub>4</sub>/water ferrofluid to improve the CO<sub>2</sub> absorption rate. The results showed that the absorption rate of CO<sub>2</sub> in Fe<sub>3</sub>O<sub>4</sub>/water ferrofluid with 0.024 vol% under magnetic field is 21% higher than the case in which no magnetic field is applied. Recently, Khani et al. [32] reported on using a magnetic field as a new technique to increase the CO<sub>2</sub> absorption in ferrofluids and reduce the pressure drop in a venturi scrubber. The study shows that under the magnetic field strength of 5120 G, increasing the nanofluid concentration from 0.01% to 0.05% led to an average increase of 20.5% in CO<sub>2</sub> removal percentage and also to the use of 0.05 vol% Fe<sub>3</sub>O<sub>4</sub>/water nanofluid under a magnetic field with different strengths, significantly increasing the CO<sub>2</sub> removal percentage in comparison with that of the distilled water. Darvanjooghi et al. [33] investigated the enhancement of the physical absorption of CO<sub>2</sub> by Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles under the influence of AC and DC magnetic fields. According to their findings, the AC magnetic field increased CO<sub>2</sub> solubility and the average molar flux of gas into the liquid phase. The diffusivity of CO<sub>2</sub> in nanofluid and the renewal surface factor increased when the magnetic field intensity increased, resulting in a decrease in diffusion layer thickness.

The use of Fe<sub>3</sub>O<sub>4</sub> particles in harvesting CO<sub>2</sub> from aqueous solutions has been a topic of interest in recent times. Pahlevaninezhad et al. [34] recently evaluated the effect of Fe<sub>3</sub>O<sub>4</sub> nanoparticles on the CO<sub>2</sub>–water mass transfer coefficient experimentally in the presence and absence of a magnetic field. This study shows that the mass transfer coefficient of CO<sub>2</sub> in water and the effective mass transfer coefficient in nanofluid were increased by up to 10% and 29% in the presence of a parallel alternative magnetic field, respectively.

Other than Fe<sub>3</sub>O<sub>4</sub> nanoparticles, the use of magnetic field effects for CO<sub>2</sub> has been studied for other systems. Razmkhah et al. [35] reported on the effect of the external field on CO<sub>2</sub> adsorption on the graphene oxide framework (GOF) studied by molecular dynamics simulation. They applied both an electric and magnetic field, parallel or perpendicular to the linker direction of the GOF and reported that there was no significant change in the GOF to CO<sub>2</sub> adsorption by a magnetic field. Another study by Zhang et al. [36] presented the performance of ammonia-based CO<sub>2</sub> adsorption under static magnetic field conditions, where the adsorption capacities were studied by a bubble reactor system. When

comparing the absorption of CO<sub>2</sub> under static magnetic field conditions and no magnetic field conditions, it was found that under the magnetic field, the absorption capacity of CO<sub>2</sub> and the removal efficiency of CO<sub>2</sub> were enhanced in ammonia-based sorbents. However, these studies presented the processes involving CO<sub>2</sub> absorption assisted by a magnetic field instead of CO<sub>2</sub> adsorption assisted by a magnetic field. Recently, the effect of magneto-water wetting on CO<sub>2</sub> adsorption has been studied theoretically by Wu et al. [37]. This study replicated the phenomena of water-cluster fragmentation and hydrogen bond creation, which was reported by molecular dynamic simulation from 0 to 10 T, enabling a quantitative study of the magneto-wetting process. These studies suggest that there is a significant effect of magnetic fields on the CO<sub>2</sub> adsorption efficiency with time.

In the current study, we report on the changes to the CO<sub>2</sub> adsorption and the structural characteristics of the magnesium-based nanocomposite under a magnetic field. Despite the widespread use of ferrofluid devices in biomedical and industrial applications, where blood or aqueous CO<sub>2</sub> levels are crucial to device efficiency, the related magneto-wetting effect for CO<sub>2</sub> collection by ferro beans has yet to be investigated. In this work, we employed an experimental technique to examine this phenomena using solid adsorbents based on MgO/Mg(OH)<sub>2</sub>. We expected that by aging samples in a magnetic field, hydrates and carbonates would form as a CO<sub>2</sub> barrier between nano-grains and slow the aging process at ambient temperature. We compare the sample data of aging under the magnetic field and without a magnetic field to hypothesize how the formation of a thin H<sub>2</sub>O layer deprives the CO<sub>2</sub> adsorption. The findings demonstrated that the amount of CO<sub>2</sub> adsorption of the samples changed under the influence of the magnetic field with time. The synthesized powder samples were characterized thoroughly using XRD, FE-SEM, BET, FTIR, and TGA analysis for their properties. The phase diagram and thermodynamic analysis were used to propose mechanisms for both thermal decomposition and CO<sub>2</sub> adsorption under the influence of a magnetic field for a prolonged time.

## 2. Materials and Methods

### 2.1. Materials

For sample synthesis, analytical grade PVA (MW 89,000–98,000, 99+% hydrolyzed) and, as the precursor, Mg(OH)<sub>2</sub> ≥99% (BioUltra) were purchased from Sigma-Aldrich (St. Louis, MO, USA). Analytical grade glacial Acetic acid (AA) 99.8% was purchased from Scharlau (Barcelona, Spain). All the chemicals were used without further purification. The water utilized in the experiments was deionized water (18 MΩ·cm).

### 2.2. Methods

The precursor solution for electrospinning was prepared by dissolving, 0.25 g of Mg(OH)<sub>2</sub> in 5 mL of acetic acid under sonication in a water bath at 50 °C for 1 h until a clear solution was obtained. After that the aqueous PVA (5% *w/w*) solution, 0.750 mL was added to the clear solution and further sonicate in a water bath at 50 °C for 5 min to eliminate any precipitation. The electrospinning was then carried out in a similar manner as we reported in our earlier study [38]. The collected layer of nanofibers was kept drying at 60 °C for 48 h for drying. The oven-dried samples were then collected as solidified flakes and calcined in a muffle furnace (Nabertherm, Lilienthal, Germany) at 300 °C for 2 h at a rate of 2 °C min<sup>-1</sup>, naturally cooling to room temperature. The samples were then ground using a motor and pestle until we obtained a fine powder. The powder sample was then separated into two parts: one kept under a magnetic field (MF) with a strength of 175 Gauss for one month at room temperature and one in room temperature with no MF for one month to observe its effect to the aging.

## 3. Characterization

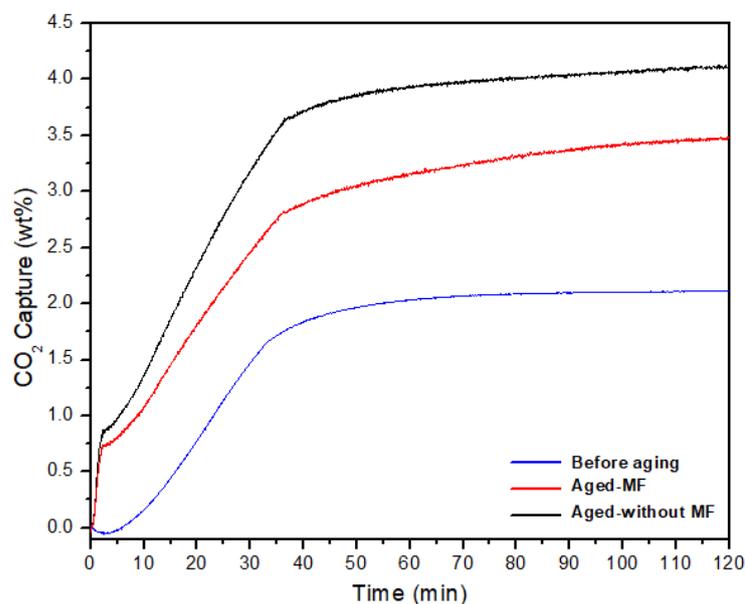
The X-ray diffraction (XRD) measurements of test samples were conducted using a D8 Advance ECO X-ray diffractometer (Bruker, Billerica, MA, USA) with Cu-K $\alpha$  radiation of 1.54 Å to evaluate powder composition and phase. The scanning angle was adjusted

between  $2\theta$  angles (from  $10^\circ$  to  $70^\circ$ ) with the X-ray generator running at the applied voltage of 40 kV and current of 25 mA. Brunauer-Emmett-Teller (BET) analysis for surface area analysis was performed by using the ASAP 2020 system (Micrometrics, Norcross, GA, USA). The BET test was conducted at  $120^\circ\text{C}$  using 0.1 g of powder samples. Fourier-transform infrared spectroscopy (FTIR) analysis was carried out using a Spectrum 2000 FTIR spectrophotometer (Perkin Elmer, Akron, OH, USA) in transmission mode ranging from  $4000$  to  $400\text{ cm}^{-1}$  with a resolution of  $1\text{ cm}^{-1}$ . Surface structure and morphology were examined by using JSM-7600F field emission-scanning electron microscopy (FE-SEM) (JEOL, Tokyo, Japan). Thermogravimetric analysis (TGA) of the samples for  $\text{CO}_2$  capture and thermal decomposition of the aged samples was conducted using a TGA Q50 analyzer (TA Instruments, New Castle, DE, USA). The thermal decomposition analysis was carried out to obtain the time-dependent weight loss profile and phase transitions during the thermal decomposition of all three samples (before age, aged no MF, and aged MF).

## 4. Results Discussion

### 4.1. Evaluation of $\text{CO}_2$ Capture Capacity

For each sample, the  $\text{CO}_2$  adsorption capacity was measured using a Q50 TGA analyzer (Figure S1). TGA analysis for  $\text{CO}_2$  adsorption was done by loading 6–7 mg of samples on to a platinum (Pt) pan in the TGA unit. Samples were first pre-treated at  $150^\circ\text{C}$  for 60 min under a flow of high purity  $\text{N}_2$  ( $40\text{ mL min}^{-1}$ ) with a ramp rate of  $10^\circ\text{C min}^{-1}$ . The temperature was then lowered to the  $30^\circ\text{C}$  at a rate of  $10^\circ\text{C min}^{-1}$  and the gas was switched from  $\text{N}_2$  to  $\text{CO}_2$  with a constant flow of pure  $\text{CO}_2$  (1 atm,  $40\text{ mL min}^{-1}$ ). The sample was analyzed at  $30^\circ\text{C}$  with a constant flow of high purity  $\text{CO}_2$  for 1.5 h as the longer time periods may not reveal any important information for practical applications [39]. Following Figure 1 shows the TGA data obtained for two samples kept under MF and one without MF.



**Figure 1.** TGA data for electrospun MgO-based nanocomposites before aging, aged under MF, and aged without MF at room temperature.

As shown in Figure 1 regarding the sample before undergoing aging at room temperature, its  $\text{CO}_2$  adsorption at room temperature was around 2.12 wt%. The TGA data in Figure 1 also shows that both samples show an increase in  $\text{CO}_2$  adsorption from their original value, yet in comparison to the  $\text{CO}_2$  capture of the sample without MF (4.13 wt%),  $\text{CO}_2$  capture of the sample under the MF (3.48 wt%) shows less adsorption value at room temperature within 90 min after 1 month of natural aging at room temperature. This result

indicates that there is an influence on CO<sub>2</sub> adsorption under an MF for a long period of time. During the aging process, due to the atmospheric exposure, the sample tends to adsorb H<sub>2</sub>O and convert MgO in to Mg(OH)<sub>2</sub> with time. However, according to Wu et al. [40], H<sub>2</sub>O molecules significantly facilitate CO<sub>2</sub> capture on MgO but not on Mg(OH)<sub>2</sub> and the formation of dehydration defects on Mg(OH)<sub>2</sub> dramatically increases the CO<sub>2</sub> adsorption energy from  $-0.045$  eV to  $-1.647$  eV. The optimized configuration of adsorbed CO<sub>2</sub> on MgO surface and Mg(OH)<sub>2</sub> surface as well as the optimized configuration in the presence of H<sub>2</sub>O molecules are shown in Figures S2 and S3.

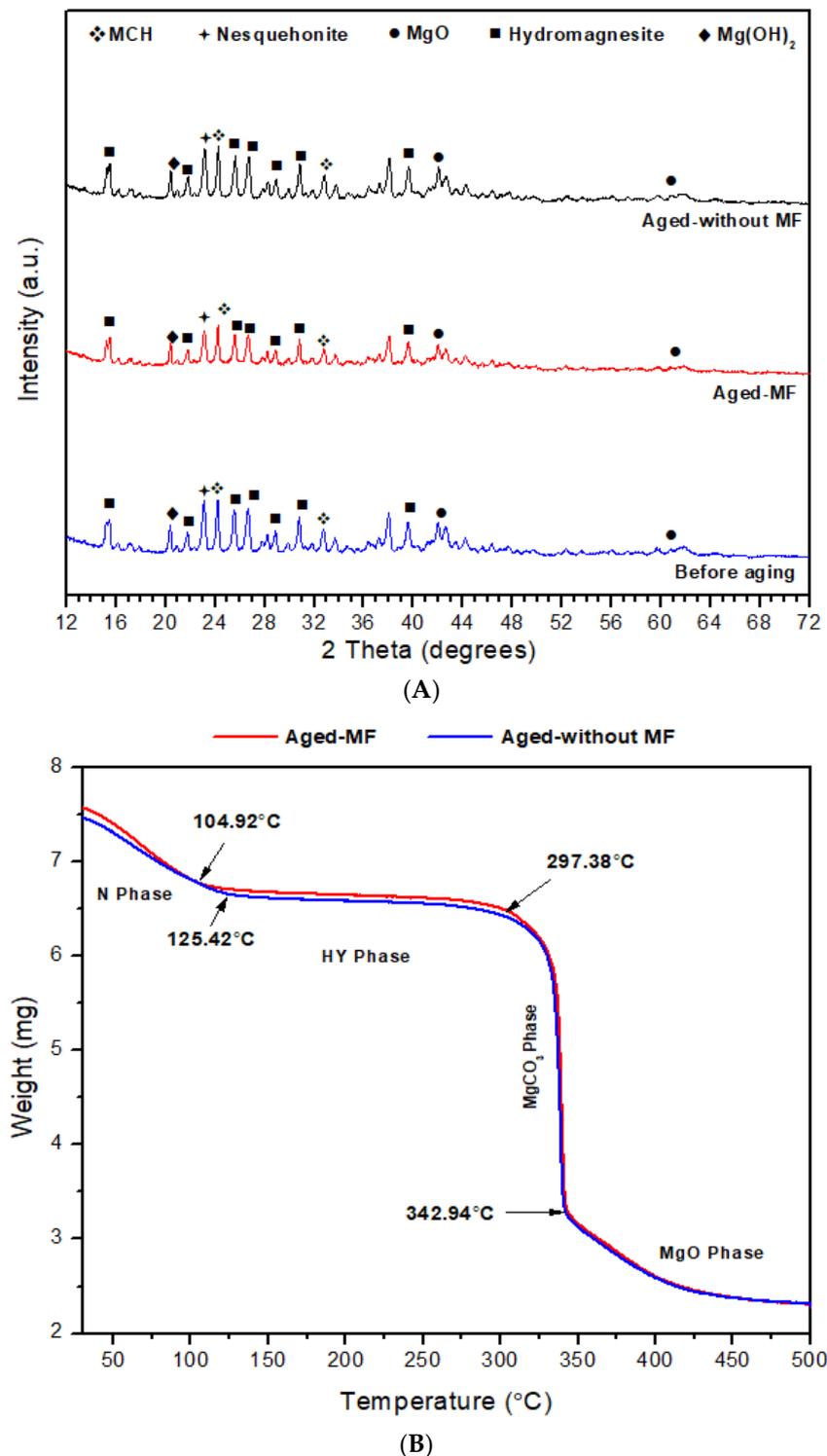
#### 4.2. Structural and Morphological Characterization

To analyze the samples' structural characteristics, XRD analysis and TGA analysis were carried out. Figure 2 presents the XRD and TGA decomposition analysis spectra for the samples before aging, after aging under MF, and under natural aging without MF for 1 month. The thermal decomposition of the samples was done using the TGA Q50 analyzer by setting the flow rate of the compressed dry air at 40 mL min<sup>-1</sup> with a ramp rate of 10 °C min<sup>-1</sup> from 30 to 500 °C. Samples (6–7 mg) were kept at 500 °C for 1 h.

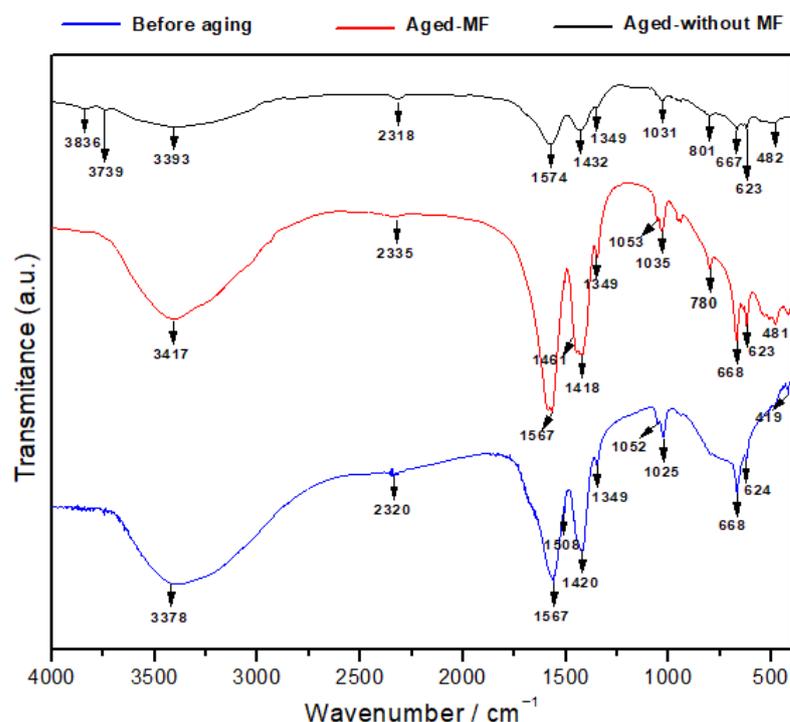
Figure 2A shows the effect on MF to the structure with aging. The main difference observed is that the peak intensities of the sample aged under MF was reduced when compared to the no-MF sample. The original sample shows the presence of magnesium oxide (MgO), magnesium hydroxide (Mg(OH)<sub>2</sub>), Nesquehonite (N) (MgCO<sub>3</sub>·3H<sub>2</sub>O), Hydromagnesite (HY) (Mg<sub>5</sub>(CO<sub>3</sub>)<sub>4</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O), and magnesium carbonate hydroxide hydroxides (MCH; Mg<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub>·3H<sub>2</sub>O). The main 2θ peaks of the MgO, namely 42.58° and 61.80°, are consistent with (200) and (220), as well with the 2θ values of the residual Mg(OH)<sub>2</sub> in 20.34°, consistent with the (001) lattice planes, which are in good agreement with MgO ICDD 01-071-6452 and Mg(OH)<sub>2</sub> ICDD 01-082-2455. Other than that, 2θ peaks of Hydromagnesite, namely 15.31°, 21.71°, 25.51°, and 41.9°, are consistent with the (011), (210), (012), and (113) lattice planes of ICDD 00-025-051. 2θ peaks of MCH 24.14°, namely 32.72° and 39.65°, are consistency with the ( $\bar{4}$ 01), (111), and (510) lattice planes of ICDD 00-006-0484. A peak related to Nesquehonite can be identified at 23.07° consistency with (002) lattice planes of ICDD 00-020-0669. Both aged with no MF and aged MF samples showed a slight peak shift in all the identified above peaks. However, the peak intensities of the sample aged under MF were less than that compared to the sample aged with no MF. A small amount of mismatch in peak positions was observed, which may have occurred due to an experimental error. Numerous other unidentified small peaks were observed in the samples, which may indicate the presence of residual polymer fragments from PVA used in electrospinning [38]. Some of the highly intensive peaks can be matched to several magnesium hydrates. However, the low intensity and large width peaks of samples can be explained by the fact that the H<sub>2</sub>O and CO<sub>2</sub> molecules are easily chemisorbed onto the sample surfaces containing MgO when aging at room temperature [41]. Senevirathna et al. [38] explained the scenario of the sample aging under natural conditions for a long period of time where the sample is a nanocomposite, comprised of monoclinic magnesium malate tetrahydrate (C<sub>8</sub>H<sub>10</sub>MgO<sub>10</sub>·4H<sub>2</sub>O) or C8, nesquehonite, and residual MgO.

Above Figure 2B shows the thermal decomposition of the aged samples under MF and without MF. According to the results, four different zones (Z1, Z2, Z3, and Z4) can be identified. The N-Phase (Z1), HY phase (Z2), MgCO<sub>3</sub> phase (Z3), and MgO phase (Z4) were identified according to previously reported data. However, the Z3 can be observed to be rather minor compared to the other zones, indicating less MgCO<sub>3</sub> in the samples. The thermal stability of the samples from 30 °C to 500 °C were obtained as Z2 > Z4 > Z1 > Z3. It was observed that for the sample aged under MF, it showed that its Z1 is in the range from 30 °C to 104.92 °C and Z2 from 104.92 °C to 297.38 °C, yet, for the sample aged without MF, it showed its Z1 from 30 °C to 125.42 °C and Z2 is in the range from 125.42 °C to 297.38 °C. For both samples, Z3 ranged from 297.38 °C to 342.94 °C and Z4 ranged from 342.94 °C to 500 °C. According to Dell and Weller [42], the initial weight loss may be due to the water loss in the N-phase and HY phases, where the HY phase has a comparatively

large decomposition, as shown in Figure 3. Above 350 °C can be an appreciable amount of CO<sub>2</sub> gas from carbonates and the residual weight reduction after 340 °C may correspond to the MgO content of N and HY [38,42]. The typical onset of decomposition of nesquehonite is from 70 °C to 100 °C and hydromagnesite is from 220 °C to 240 °C [43], which confirms the presence in the above Figure 2A,B, wherein XRD data confirms the presence.



**Figure 2.** (A) XRD patterns for electrospun MgO-based nanocomposites, as prepared, after aging under MF and aging not under MF. (B) The thermal decomposition during the aging process under MF and no MF at room temperature.



**Figure 3.** FTIR spectra for the samples as prepared: aging under MF and aging under no MF at room temperature.

The FTIR analysis for the samples was carried out to obtain additional information on their chemistry and structure, as shown in Figure 3. From FTIR analysis, the stretching vibration mode for the Mg–O–Mg compound was seen in the range of 481–668  $\text{cm}^{-1}$ , which is similar to what was reported in Balamurugan et al. [44] and Mohandes et al. [45] as strong and broad peaks in all three samples, while the as-prepared sample showed sharper and more intensive peaks than others. The sample under natural aging with no MF applied shows broader peaks for the stretching vibration mode for the Mg–O–Mg [44–46]. The stretching vibration of the O–H of water molecules and surface hydroxyl groups give rise to broad band in the region between 3378  $\text{cm}^{-1}$ , 3417  $\text{cm}^{-1}$ , and 3393  $\text{cm}^{-1}$  in all three samples, yet the similar sample aged without MF shows a broad and less intensive peak related to the O–H stretching vibration (3393  $\text{cm}^{-1}$ ) [47]. Two distinct bands are seen in the before-aging sample (1052  $\text{cm}^{-1}$  and 1025  $\text{cm}^{-1}$ ), aged sample under MF (1053  $\text{cm}^{-1}$  and 1035  $\text{cm}^{-1}$ ), and aged sample without MF (1031  $\text{cm}^{-1}$  and 1024  $\text{cm}^{-1}$ ), which are attributed to the bending vibration of adsorbed water [44]. The peak intensity was reduced in the natural aged sample with no MF and increased the aged sample under MF, indicating more O–H formation. The difference is mainly due to the aerial adsorption of water molecules onto the MgO-based surfaces when they are exposed to the atmosphere where the sample under MF adsorbed more compared to the other two. The adsorption peak seen at the wavenumbers 1420  $\text{cm}^{-1}$ , 1418  $\text{cm}^{-1}$ , and 1432  $\text{cm}^{-1}$  in all three samples can be assigned to the asymmetric stretching of the carbonate ion, which is of the  $\text{CO}_3^{2-}$  species [47]. In addition, a weak band corresponding to the adsorption of gas-phase  $\text{CO}_2$  is visible at 2320  $\text{cm}^{-1}$ , 2335  $\text{cm}^{-1}$ , and 2318  $\text{cm}^{-1}$  in all three samples [48,49]. However, the sample with natural aging with no MF applied shows weakened bonds. When compared to the fresh sample, due to the  $\text{CO}_3^{2-}$  chemisorption with natural aging, a shift is observed towards the higher wavenumbers [41]. Interestingly, the peak intensity of all the peaks identified are reduced in the natural-aged sample with no MF. The peak at 1567  $\text{cm}^{-1}$  and 1574  $\text{cm}^{-1}$  is attributable to the influence of the C=O vibration of  $\text{CO}_3^{2-}$  [49], where the aged-under-MF sample shows an intensive peak compared to the no-MF sample, indicating that under MF, the formation of  $\text{CO}_3^{2-}$  increased in the sample.

### 4.3. Morphology Analysis

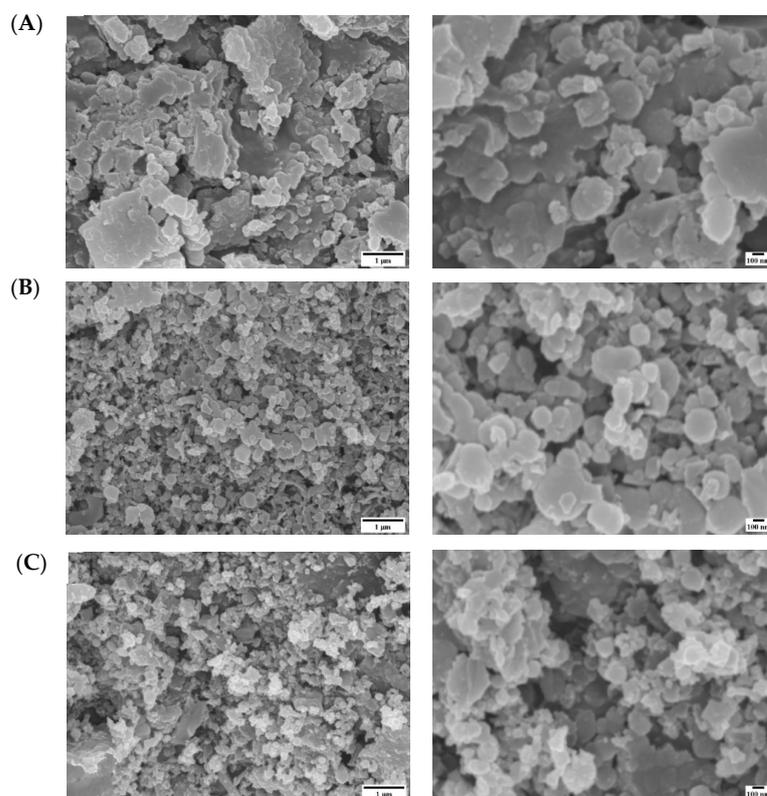
In order to have an idea of the effect on the surface area of the samples under MF, BET analysis was carried out. The surface area and pore volume parameters of samples are shown in Table 1.

**Table 1.** Effect of MF for surface area and pore volume parameters of samples.

Sample	Surface Area (m <sup>2</sup> /g)	Total Pore Volume (cm <sup>3</sup> /g)	Avg Pore Size (nm)
As prepared	12.45	0.359	115.60
Aged no MF	79.52	0.069	3.48
Aged under MF	25.62	1.389	216.93

The synthesized samples had a higher pore volume but less surface area before aging at room temperature. In particular, the BET surface area reached as high as 79.52 m<sup>2</sup>/g when it aged without MF for 1 month at ambient conditions, yet it recorded the lowest pore size as 3.48 nm. When compared with the sample aged with no MF, the sample aged under MF shows a lesser surface area of 25.62 m<sup>2</sup>/g, yet it shows a higher pore size of 216.93 m<sup>2</sup>/g. This result indicates that there is an effect of the MF to the sample's microstructure. This result can be validated using the TGA results obtained where the highest CO<sub>2</sub> adsorption at room temperature was recorded for the sample aged without MF, which records the high BET surface area of the three samples.

The surface analysis of the samples was carried out using SEM analysis. Figure 4 presents the SEM images obtained for three samples.



**Figure 4.** SEM images for (A) sample as prepared. (B) Sample aged under no MF. (C) Sample aged under MF for 1 month at room temperature. Right side indicates low magnification and left side high magnification.

All the samples show sheet like structures, yet the aged samples show more uniform and smooth structures at the nanoscale features, varying from 100–200 nm.

## 5. Discussion

Based on the data collected following Figure 5, we summarize the mechanism to explain the relationship of our sample with aging under MF and without MF. H<sub>2</sub>O molecules govern the volume ratio between CO<sub>2</sub>-phobic (Mg(OH)<sub>2</sub>) and CO<sub>2</sub>-philic (MgO) grains, and the total volume of Mg(OH)<sub>2</sub> rises as the quantity of H<sub>2</sub>O molecules grows according to prior density-functional theory (DFT) calculations [40]. Additional H<sub>2</sub>O molecules may precipitate between the MgO and Mg(OH)<sub>2</sub> grains due to magneto-wetting in this work, forming H<sub>2</sub>O thin films that inhibit CO<sub>2</sub> molecules from diffusing between the MgO and Mg(OH)<sub>2</sub> grain boundaries, which is consistent with the aforementioned notion. As a result, the popular belief that the magneto-water-wetting effect increases the CO<sub>2</sub> collection efficiency of diverse nanofluids is incorrect.

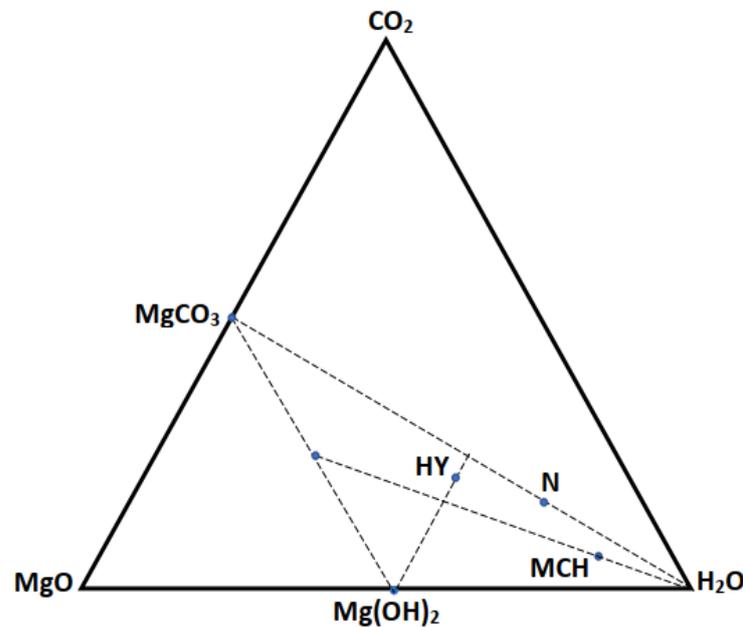


Figure 5. Phase relationship for the studied system.

The control mechanism of magnetic radiation is the formation of an H<sub>2</sub>O film on the surface of pores due to the magneto-wetting [37]. This H<sub>2</sub>O film hinders the diffusion of vapor-H<sub>2</sub>O into the lattice and slows the hydration of the powder during the aging process. The as-prepared powder sample is located along the MgO to H<sub>2</sub>O line in Figure 5. However, with prolonged aging, it goes towards MgCO<sub>3</sub>, which quickly formed at 342.94 °C (Figure 3). The Z2 zone has a long temperature range to form HY, which may be due to the formation of MCH and N simultaneously (Figure 2B). After 125.42 °C, MCH and N form. For continuous aging, the sample may follow the line linking MCH, N, and CO<sub>2</sub> in the diagram in Figure 5. It has been established that the MF could affect the physicochemical properties of water [50–53] as, under the MF, water molecules become magnetized. Han et al. [54] reported on the effect of MF on the optical property states that the spiral motion of ions is imposed to the water molecules due to the MF. Holysz et al. [51] concluded that MF may increase the electrolyte conductivity due to the decrease in ion radius. Fujimura and Iino [55] reported on an increase in surface tension with an increase of MF due to the stabilization of hydrogen bonds. The surface tension increases when the bulk Helmholtz free energy increases due to the stabilized hydrogen bonds. As the sample ages at room-temperature conditions, atmospheric H<sub>2</sub>O and CO<sub>2</sub> molecules tend to adsorb the samples, resulting in a change in the samples over time [38]. Cai et al. [52] reported that the water intramolecular energy decreased, and activation energy increased over the exposure time of MF to the sample, and the results suggested that more hydrogen bonds were formed, and the mean size of water clusters got larger by magnetic field treatments to

the samples. Therefore, due to these arrangements, more H<sub>2</sub>O molecules tend to adsorb into sample under the MF, resulting in H<sub>2</sub>O molecules blocking the pores and leading to the relative decrease in CO<sub>2</sub> adsorption in comparison with the aged samples without MF. This can also promote the formation of carbonates in the samples, hence hindering the adsorption (Figure 2A).

## 6. Conclusions

The effect of magneto-wetting on CO<sub>2</sub> adsorption was experimentally investigated using nano-MgO/Mg(OH)<sub>2</sub>-based materials. Ambient H<sub>2</sub>O contributes to the Mg(OH)<sub>2</sub> nucleation and growth process in a MgO/Mg(OH)<sub>2</sub> composite during normal aging. However, when an MF is present, the Mg(OH)<sub>2</sub> growth process is accelerated and additional H<sub>2</sub>O molecules may be trapped between the grains of MgO and Mg(OH)<sub>2</sub> to further impede CO<sub>2</sub> diffusion. We demonstrated that, contrary to popular belief, magneto-water-wetting does not always increase CO<sub>2</sub> adsorption; in fact, when Mg(OH)<sub>2</sub> predominates in the nanocomposite, CO<sub>2</sub> adsorption might actually decrease. As a result, the impact of MF on CO<sub>2</sub> adsorption is critical. These discoveries might lead to applications such as extending the life of CO<sub>2</sub> adsorbents and controlling the hydration process at room temperature. The findings might be used to design and develop new nanofluid devices for medical and industrial applications in which blood CO<sub>2</sub> levels are critical for device efficiency.

**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/ma15030983/s1>, Figure S1: A schematic diagram of the TGA analysis process for the CO<sub>2</sub> capture capacity of the samples and figure of TGA Q50 analyser [1]; Figure S2: Optimized configuration of adsorbed CO<sub>2</sub> on MgO surface (a) and with H<sub>2</sub>O (b). Atoms are shown as colored balls: hydrogen (white), oxygen (red), magnesium (green), and carbon (grey); Figure S3: Optimized configuration of adsorbed CO<sub>2</sub> on Mg(OH)<sub>2</sub> surface (a) and with H<sub>2</sub>O (b). Atoms are shown as colored balls: hydrogen (white), oxygen (red), magnesium (green), and carbon (grey).

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