Low carbon dioxide partial pressure capture in organic biomass matter

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**Abstract**

For carbon dioxide (CO2) capture, adsorption-based technologies have attracted increasing interest because of low cost, high efficiency and reliability. The identification of a sustainable resource for appropriate adsorbent is a trial-and-error experiment and costly. Therefore, high-throughput computational methods are considered for efficient adsorbent design.

Organic biomass matter (biomass hereinafter) can be considered as a sustainable and cheap resource for adsorptive capture of CO2. Biomass is one of the most abundant raw material on the earth. Therefore, we investigated CO2 capture and underlying molecular mechanisms using molecular modeling over a wide range of biomass microstructure.

We discovered for the first time that CO2 adsorption in biomass is governed by a ‘CO2–water–biomass’ network that interacting through sharing common water molecule. The water–CO2 interactions are through CO–OH and the same water molecule participates in water–biomass interaction through H–OH or HO–H. We showed regulatory role of biomass moisture content in CO2 admission. Our finding explains on demand carbon dioxide uptake and release by altering moisture content. We found capacitates of 5–56gram CO2 per gram biomass are achievable at ambient conditions i.e. temperature range of 230–310 K and atmospheric pressure, 1 bar.

**Keywords**: biomass; carbon dioxide; gas adsorption; CO2 capture; greenhouse gas control

#### Introduction

In environmental pollution related works, addressing air pollution with greenhouse gases such as carbon dioxide has been subject of intensive researches ([Asgarpour Khansary, Marjani, & Shirazian, 2017](#_ENREF_4); [Mehmood et al., 2018](#_ENREF_48)). Carbon dioxide (CO2) has potential applications in industries such as enhanced oil recovery, food and beverage manufacturing, pulp and paper manufacturing, metal fabrication and etc. ([Chauvy, Meunier, Thomas, & De Weireld, 2019](#_ENREF_12); [Jieyun Jiang, Rui, Hazlett, & Lu, 2019](#_ENREF_32)). Such applications make CO2 capture a must. CO2 is also major compounds involved in global warming ([Galashev, 2011](#_ENREF_23)). Therefore low cost and efficient technology development for capture and remediation of greenhouse gases is of urgent demands of our society ([Leung, Caramanna, & Maroto-Valer, 2014](#_ENREF_43)).

For CO2 capture and storage, a number of technologies have been introduced including amine-based operations, adsorption, membrane technologies, metal-organic frameworks and etc.([Kumar et al., 2018](#_ENREF_39); [MacDowell et al., 2010](#_ENREF_46)). Adsorption-based technologies have attracted increasing interest among others due to low cost, efficiency, and reliability ([Kerry, 2007](#_ENREF_37)).

In adsorption processes, gases are selectively adsorbed onto the surface of adsorbents either physically or chemically ([Yang, 2013](#_ENREF_62)). Thus, the physicochemical properties of adsorbent including surface area, porosity, surface texture, and particularly active sites affect adsorbent performance ([Dąbrowski, 2001](#_ENREF_17)). Therefore there has been an ever-increasing interest in material search and screening for adsorbent ([Pevida et al., 2008](#_ENREF_52)) in order to address global challenge of reducing gaseous pollutants emission ([Jingjing Jiang, Ye, & Liu, 2019](#_ENREF_33)).

The initial feasibility/suitability estimation/analysis is a required step for adsorbent selection ([H. Li, Yan, Zhang, & Lichtfouse, 2019](#_ENREF_44)). The selection of the candidate adsorbent is a trial-and-error experiment which in turn is costly and uses much resources and requires facility maintenance ([Ali Aroon & Khansary, 2017](#_ENREF_1)). To avoid trial-and-error, the application and development of high-throughput computational methods have been considered for efficient adsorbent design ([Hergert, Ernst, & Däne, 2004](#_ENREF_30)). Such as our recent review of polymeric adsorbents for CO2 capture ([Asgarpour Khansary et al., 2017](#_ENREF_4)) where we also introduced a predictive method to assist engineering practices in industry for uptake estimations.

For instance, Gómez-Pozuelo et al. ([Gómez-Pozuelo et al., 2019](#_ENREF_26)) synthesised 23 different amino-modified sorbents by grafting and impregnation for CO2 capture. They found that CO2 uptakes as high as 61.3 and 67.1 mili gram (mgr) CO2 per gram (gr) adsorbent is achievable respectively for grafted and impregnated samples under dry conditions i.e. 45 °C and 1 bar. The best achievable adsorption capacity was 67.1 mgr CO2/gr adsorbent. They observed that CO2 uptake enhancement when the fed gas contains water/moisture. In another work by Azzouz et al. ([Azzouz et al., 2010](#_ENREF_6)), a number of different montmorillonite samples intercalated with polyol dendrimers were synthesized and CO2 uptake ranging between 22 and 110 mgr CO2/gr adsorbent was reported. Kutorglo et al. ([Kutorglo et al., 2019](#_ENREF_40)) synthesised nitrogen-rich hierarchically porous polyaniline-based adsorbents. Their investigation on CO2 capture, performed at 273.15 K and 1 bar, showed a capture capacity of optimum material as 402.25 mgr CO2/gr adsorbent. Guo et al. ([Guo, Zhao, Sun, Li, & Lu, 2018](#_ENREF_27)) synthesized silica aerogel supported K2CO3 sorbents with different K2CO3 loadings and examined their CO2 capture performances using a simulated ultra-dilute CO2 flue gas stream (1.0% CO2). They reported CO2 uptake as high as 58.09 mgr CO2/gr sorbent at 20 °C. Zhao et al. ([Zhao et al., 2018](#_ENREF_65)) examined mesoporous MgO promoted by NaNO3/NaNO2 for CO2 capture at 350 °C in the presence of 0.85 bar of CO2. They reported a CO2 capture capacity as high as 871.398 mgr CO2/gr sorbent. Zhang et al. ([S. Zhang, Chen, & Ahn, 2019](#_ENREF_64)) reviewed amine-functionalized silica for CO2 capture. They concluded that capture capacities are below 200 mgr CO2/gr adsorbent. They also found that for polyacrylonitrile nanoparticle‐derived hierarchical structure, the average CO2 adsorption capacity is 156.67 mgr CO2/kg adsorbent at 0 °C and 1 atm ([Beltzung et al., 2018](#_ENREF_8)). In an attempt to impregnate carbon nanotubes by using polyethylenimine, Keller et al. ([Keller et al., 2018](#_ENREF_36)) achieved a maximum CO2 uptake of 93 mgr CO2/gr sorbent. Parvazinia et al. ([Parvazinia, Garcia, & Maroto-Valer, 2018](#_ENREF_51)) reported the use of ion exchange resins as amine functionalized CO2 adsorbents at 25 °C. They achieved capacities around 77.01 mgr CO2/gr adsorbent. Chiang et al. ([Chiang, Yeh, & Weng, 2019](#_ENREF_13)), synthesized activated carbon fibers based on polyacrylonitrile which was modified by using potassium hydroxide and tetraethylenepentamine. They performed CO2 uptake experiments at 1 atm and 25 °C. They reported a CO2 capture capacity of 120.58 mgr/gr adsorbent. Qin et al. ([Qin et al., 2019](#_ENREF_53)) synthesized nitrogen-doped asphaltene-based porous carbon nanosheet. They examined the carbon dioxide capture capacity of these materials and found CO2 adsorption capacity of 176.04 mgr/gr at 25 °C and 1 bar and 242.055 mgr/gr at 0 °C and 1 bar. Sevilla et al. ([Sevilla & Fuertes, 2011](#_ENREF_55)) examined starch and cellulose and sawdust for their carbon dioxide capture capacity by chemical activation. They reported CO2 uptake capacity as high as 212 mgr CO2/gr adsorbent at room temperature i.e. 25 °C. Coromina et al. ([Coromina, Walsh, & Mokaya, 2016](#_ENREF_15)) synthesized a series of activated carbons from the biomass raw materials Jujun grass and Camellia japonica using hydrothermal carbonization. They reported CO2 uptake capacity of up to 66.015 mgr/gr adsorbent at 25 °C and 0.15 bar and CO2 uptake capacity of 220.05 mgr/gr adsorbent at 25 °C and 1 bar. Li et al. ([Q. Li et al., 2010](#_ENREF_45)) synthesized mesoporous carbon enriched in nitrogen using ethylenediamine and carbon tetrachloride. They measured CO2 uptake capacity of obtained material at 25 °C and 1 atm and reported adsorption capacity of 127.629 mgr/gr adsorbent. Hao et al. ([Hao, Li, Qian, & Lu, 2010](#_ENREF_28)) used L-lysine to synthesize porous carbon monolith and measured CO2 uptake capacity of obtained material at 25 °C and 1 atm and reported adsorption capacity of 137.7513 mgr/gr adsorbent. Song et al ([Song, Shen, Wang, & Fan, 2014](#_ENREF_56)) synthesized a number of nitrogen-containing granular porous carbons from poplar anthers and measured its CO2 capacity at 50 bar and 25 °C. They reported adsorption capacity of 2257.713 mgr/gr adsorbent. Fujiki and Yogo ([Fujiki & Yogo, 2016](#_ENREF_22)) used alkali carbonates for chemical activation of chitosan and synthesized highly porous nitrogen-doped activated carbons. They reported a CO2 adsorption capacity of 70.416 mgr/gr adsorbent at 25 °C and 15 kPa and 215.649 mgr/gr adsorbent at 25 °C and 100 kPa. Parshetti ([Parshetti, Chowdhury, & Balasubramanian, 2015](#_ENREF_50)) used empty fruit bunch of oil palm trees to synthesized microporous carbon materials and reported CO2 uptake capacity of 163.2771 mgr/gr adsorbent at 25 °C and at a pressure of 1 atm. Wei et al. ([Wei et al., 2012](#_ENREF_61)) through KOH activation prepared adsorbents for CO2 capture from bamboo. They reported CO2 uptakes up to 308.07 mgr/gr adsorbent at 273 K and 1 bar.

Here, we candidate organic biomass matter (hereinafter biomass) as a potential adsorbent for CO2 uptake and capture in ambient conditions. We are interested in ambient conditions because it would not involve operational difficulties and additional utilities, which in turn means very low fixed/installation costs and maintenance requirements. Biomass pile up on the ground surface and form the upper layer of many suburb areas such as farms, jungles, etc. ([Bajpai, 2017](#_ENREF_7)). Biomass is the most freely abundant material available on the earth ([Asgarpour Khansary & Shirazian, 2016](#_ENREF_5)). Thus biomass can be considered as a sustainable, cheap, accessible and environmentally friendly resource for a wide range of applications ([García-Condado et al., 2019](#_ENREF_24)). Biomass is mostly composed of carbohydrate polymers such as cellulose and hemicellulose and aromatic polymer like lignin. Biomass possess a wide variety of functional groups and is able to interact with a wide range of materials ([Anastopoulos et al., 2019](#_ENREF_2); [Edris Karezani, Hallajisani, & Asgarpour Khansary, 2017](#_ENREF_34)). For instance, biomass has found many industrial applications in pulp and paper industry, biofuel (bioethanol) production, adsorptive water treatment and so on ([Magalhães Jr et al., 2019](#_ENREF_47)).

Our suggestion is made mainly based on the resource sustainability and presence of wide range of functional groups in biomass constitutional components. As far as we know, it is the first time the application of biomass for CO2 capture at ambient conditions, particularly low pressures, has been investigated. In order to judge the applicability of biomass as a CO2 adsorbent, it is required to understand (1) mechanisms by which the CO2 can be admitted to biomass and (2) the biomass capacity to capture CO2. Thus, we examined the mechanisms and capacity of biomass for CO2 adsorption by computational experiments. We tried to analysis the CO2 admission into a wide variety of biomass samples so that the conclusions could be comprehensive. Special attention was given to the molecular level factors governing the CO2 admission.



#### Experimental

## Preparation of model structures

Biomass is mainly composed of lignin, cellulose and hemicellulose ([Chung & Washburn, 2016](#_ENREF_14)). The biomass composition and microstructure depends on the origin and geographical location of biomass ([Chung & Washburn, 2016](#_ENREF_14)) as listed in Table 1. These data were used to construct biomass models using Amorphous Cell module of Material Studio computational package. The convergence tolerances are energy: 2.0×10-5 kcal/mol, force: 10-3 kcal/mol/Å, max iterations: 104, displacement: 10-5 Å. The repeating unit structures of lignin, cellulose and hemicellulose were retrieved from our previous works ([Ghasemi, Asgarpour Khansary, Marjani, & Shirazian, 2017](#_ENREF_25); [E. Karezani, Hallajisani, & Khansary, 2017](#_ENREF_35)). Our cellulose and hemicellulose models were constructed as 15 times of their corresponding repeating units, and for lignin, one repeating unit was used, particularly to keep computational costs in a reasonable range. These structures were first relaxed i.e. geometrically optimized and energetically minimized using INTERFACE force field model v.1.5, the details of force field can be found in the reference work of Heinz et al. ([Dharmawardhana et al., 2017](#_ENREF_19); [Heinz, Lin, Kishore Mishra, & Emami, 2013](#_ENREF_29)). The relaxations were carried out using Forcite module as implemented in Material Studio computational package.

Table 1. List of biomass sources and their composition ([Shurong Wang, Dai, Yang, & Luo, 2017](#_ENREF_59)) used in this work

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Biomass source** | | **Content (w.t. %)** | | |
| *No.* | *Source* | *Type* | *Cellulose* | *Hemicellulose* | *Lignin* |
| 1 | Alder | Hardwood | 45.5 | 20.6 | 23.3 |
| 2 | Aspen | Hardwood | 52.7 | 21.7 | 19.5 |
| 3 | Bamboo | Herbaceous and agricultural | 39.8 | 19.49 | 20.81 |
| 4 | Beech1 | Hardwood | 45 | 33 | 20 |
| 5 | Beech2 | Hardwood | 44.2 | 33.5 | 21.8 |
| 6 | Cherry wood | Hardwood | 46 | 29 | 18 |
| 7 | Corn cob | Herbaceous and agricultural | 34.61 | 15.24 | 18.16 |
| 8 | Corn leaves | Herbaceous and agricultural | 26.93 | 13.27 | 15.18 |
| 9 | Corn straw | Herbaceous and agricultural | 42.7 | 23.2 | 17.5 |
| 10 | Eastern Red cedar | Softwood | 40.3 | 17.9 | 35.9 |
| 11 | Fir | Softwood | 45 | 22 | 30 |
| 12 | Hazelnut shell | Herbaceous and agricultural | 25.2 | 28.2 | 42.1 |
| 13 | Japanese beech | Hardwood | 43.9 | 28.4 | 24 |
| 14 | Japanese cedar | Softwood | 38.6 | 23.1 | 33.8 |
| 15 | Miscanthus | Herbaceous and agricultural | 34.4 | 25.4 | 22.8 |
| 16 | P.armandii Franch | Softwood | 48.4 | 17.8 | 24.1 |
| 17 | Pine | Softwood | 46.9 | 20.3 | 27.3 |
| 18 | Poplar | Hardwood | 49 | 24 | 20 |
| 19 | Rice husk | Herbaceous and agricultural | 37 | 23.43 | 24.77 |
| 20 | Rice straw1 | Herbaceous and agricultural | 37 | 16.5 | 13.6 |
| 21 | Rice straw2 | Herbaceous and agricultural | 34.53 | 18.42 | 20.22 |
| 22 | Spruce1 | Softwood | 45.6 | 20 | 28.2 |
| 23 | Spruce2 | Softwood | 43 | 29.4 | 27.6 |
| 24 | Switch grass | Herbaceous and agricultural | 40–45 | 31–35 | 6–12 |
| 25 | Wheat straw | Herbaceous and agricultural | 37.55 | 18.22 | 20.24 |
| 26 | Willow | Hardwood | 41.7 | 16.7 | 29.3 |

We relaxed all the biomass models generated by Amorphous Cell module using INTERFACE force field model v.1.5 ([Dharmawardhana et al., 2017](#_ENREF_19); [Heinz et al., 2013](#_ENREF_29)) employing convergence tolerances as energy: 2.0×10-5 kcal/mol, force: 10-3 kcal/mol/Å, max iterations: 104, displacement: 10-5 Å. To get lowest energy structures and avoiding local energy minimum configurations, the relaxed structures were exposed to five consecutive annealing cycles up to 500 K for 75ps. Then, to ensure reaching true equilibrium structures, the structures were exposed to molecular dynamics in constant number of molecules, pressure and temperature (NPT) ensemble over a wide temperature range of 230 – 310 K at atmospheric pressure, 1 bar for a period of 75ps followed by another 75ps dynamic run in constant number of molecules, volume and energy (NVE) ensemble ([Černý, 1985](#_ENREF_11); [Kirkpatrick, Gelatt, & Vecchi, 1983](#_ENREF_38)). The velocity Verlet algorithm is used for integration of Newton’s equation with the utilization of Berendsen thermostat ([Lemak & Balabaev, 1994](#_ENREF_41)). These calculations were performed using Frocite module in Material Studio computational package.

We noted that the naturally available biomass may contain slight amount of moisture, therefore we created wet biomass models by adding water. It is worthy to mention that the water (as well as CO2) structure is retrieved from National Institute of Standards and Technology (NIST) chemistry webbook available at <https://webbook.nist.gov/chemistry/>. We generated biomass samples with up to 2.5 w.t. % water content (relative mass humidity). It is worthy to mentioned that due to the simultaneous presence of CO2 and H2O, it was suspected that these molecules might participate in formation reactions of carbonic acid ([Andersen, 2002](#_ENREF_3)). However, as dictated by the hydration equilibrium constant of carbonic acid, approximately 0.0017 at 25 °C carbon dioxide will remain mostly as CO2 molecules ([X. Wang, Conway, Burns, McCann, & Maeder, 2010](#_ENREF_60)).

The generated wet biomass models were also relaxed using INTERFACE force field model ([Dharmawardhana et al., 2017](#_ENREF_19); [Heinz et al., 2013](#_ENREF_29)) employing convergence tolerances as energy: 2.0×10-5 kcal/mol, force: 10-3 kcal/mol/Å, max iterations: 104, displacement: 10-5 Å. The relaxed structures were exposed to five consecutive annealing cycles up to 500 K for 75ps followed by 75ps long molecular dynamics in NPT ensemble and another 75ps molecular dynamics in NVE ensemble ([Černý, 1985](#_ENREF_11); [Kirkpatrick et al., 1983](#_ENREF_38)). The velocity Verlet algorithm is used for integration of Newton’s equation with the utilization of Berendsen thermostat ([Lemak & Balabaev, 1994](#_ENREF_41)). All these calculations were performed using Forcite module in Material Studio computational package.

## CO2 uptake in biomass

At ambient conditions as considered in this work i.e. temperature range of 230 – 310 K and atmospheric pressure, 1 bar, the Henry law governs the transfer of any component between two phases in contact ([Leng et al., 2015](#_ENREF_42)). For calculation of Henry constants, we used Sorption module of Material Studio computational package. The Henry constant is given as  ([Bezus, Kiselev, Lopatkin, & Du, 1978](#_ENREF_9)), where *V* is the volume of biomass model, *β* is the reciprocal temperature i.e. , where *kB* =1.38064852×10-23 *J*/*K* is the Boltzmann constant, *T* is the absolute temperature in Kelvin, *Em* is the total energy of configuration *m* comprised as sum of (i) the intermolecular energy between the carbon dioxide molecules, (ii) the interaction energy between the carbon dioxide molecules and the biomass and (iii) the total intramolecular energy of the carbon dioxide molecules which is the sum of the intramolecular energy of all carbon dioxide molecules itself. *μintra* is the intramolecular chemical potential given as  where the average is taken over a uniform ensemble ([Frenkel & Smit, 2002](#_ENREF_21)). Sorption module in Material Studio computational package, which we used here for our calculations, employs configurational bias Monte Carlo technique to search configurational space according to a simulated annealing schedule ([Černý, 1985](#_ENREF_11); [Kirkpatrick et al., 1983](#_ENREF_38)). Each configuration, in this context, then could have a probability as given by  where *C* is an arbitrary constant.

For all biomass samples, the Henry constants were determined by following above-mentioned approach over a wide temperature range of 230 – 310 K and at atmospheric pressure (1 bar). Then the CO2 molecules were added to each corresponding biomass model. All these CO2-containing biomass models then were relaxed using INTERFACE force field model ([Dharmawardhana et al., 2017](#_ENREF_19); [Heinz et al., 2013](#_ENREF_29)) employing convergence tolerances as energy: 2.0×10-5 kcal/mol, force: 10-3 kcal/mol/Å, max iterations: 104, displacement: 10-5 Å. To make sure that these configurations are equilibrium structures and not local optimal ones, we exposed the relaxed structures to five consecutive annealing cycles up to 500 K for 75ps followed by 75ps long molecular dynamics in NPT ensemble and another 75ps dynamic run in NVE ensemble ([Černý, 1985](#_ENREF_11); [Kirkpatrick et al., 1983](#_ENREF_38)). The velocity Verlet algorithm is used for integration of Newton’s equation with the utilization of Berendsen thermostat ([Lemak & Balabaev, 1994](#_ENREF_41)).

#### Results and discussion

In order to examine the capacity of biomass for CO2 capture and the underlying molecular mechanisms, we used molecular modeling technique. We performed computational experiments over a wide temperature range of 230 – 310 K at atmospheric pressure, 1 bar. We tried to analysis the CO2 admission into a wide variety of biomass samples so that the conclusions could be comprehensive.

## CO2 uptake capacity

The details of relaxed dry (no water molecule) biomass models are listed in supplementary file. For each biomass model in our work, after relaxation and molecular dynamic simulations, the remained CO2 molecules were counted and the amount of CO2 molecules admission into each biomass models were determined as. To convert to , one can divide it by with , where *ρ* is the biomass density in gr/cc. Our calculated capacities are reported in Fig.1.

**dry**

**0.03 w.t. %**

**2.5 w.t. %**

**1.0 w.t. %**

**CO2 molecules / [(kPa.Å3)-1] biomass**

Fig.1. CO2 uptake capacity averaged over all various biomass models calculated over a wide temperature range and moisture contents at atmospheric pressure. Increasing temperature and moisture content, the CO2 admission capacity decreases in all biomass models which is in agreement with the characteristics of adsorption process.

From Fig.1, it can be readily seen that by increasing the temperature, the CO2 admission capacity decreases in all biomass models. Our results are in agreement with the temperature dependency and characteristics of adsorption process ([Crittenden & Thomas, 1998](#_ENREF_16)). Increasing the moisture content decreases the capacity of all biomass models. Sorption capacity of the biomass reduces with increase in its wetness (Fig.1). This is due to the fact that higher moisture content results in saturation of internal pores and leaves less rooms for CO2 to enter ([Bowen, 2011](#_ENREF_10); [Forzieri, Alkama, Miralles, & Cescatti, 2017](#_ENREF_20)). This results in lower CO2 update at higher moisture contents as it can be seen in Fig.1. By analysis of trajectories, we found that water molecules play a two-fold role. While higher content of moisture reduces the uptake capacity, but moisture establishes new interactions with CO2 and biomass molecules. These interactions trap CO2 and restrict CO2 movement. This in turn results in sustaining the captured CO2 in presence of water molecule. Biomass can bring the opportunity for a low cost and sustainable CO2 capture with a capacity around 50 gr CO2/gr biomass.

## Underlying molecular mechanisms

In order to discover the underlying interplay of water, CO2 and biomass, we analysed obtained trajectories. We found that water molecules interact with CO2 molecules through the CO2–OH interactions. These interactions add a constraint to hold CO2 molecules within biomass pores. Such trapping role of water for CO2 molecules has been observed also in previous water–CO2 research works ([Serre et al., 2007](#_ENREF_54)) reporting that a cage of forty-six water molecules is able to trap a maximum of eight CO2 molecules through CO–OH interactions. We observed in trajectories that the same water molecule – which interacted with CO2 – interacts with biomass either (i) though its oxygen in OH group and a hydrogen on biomass molecules or (ii) its hydrogen (not is the same OH group) and an oxygen on biomass molecules. These interactions are illustrated in Fig.2. This creates a ‘CO2–water-biomass’ network of interactions sharing common water molecules which we suggest as the underlying interplay of water, CO2 and biomass in CO2 uptake and capture by biomass.

water interacting with CO2 through its OH group and in meanwhile interacting with oxygen in biomass

Sample trajectory

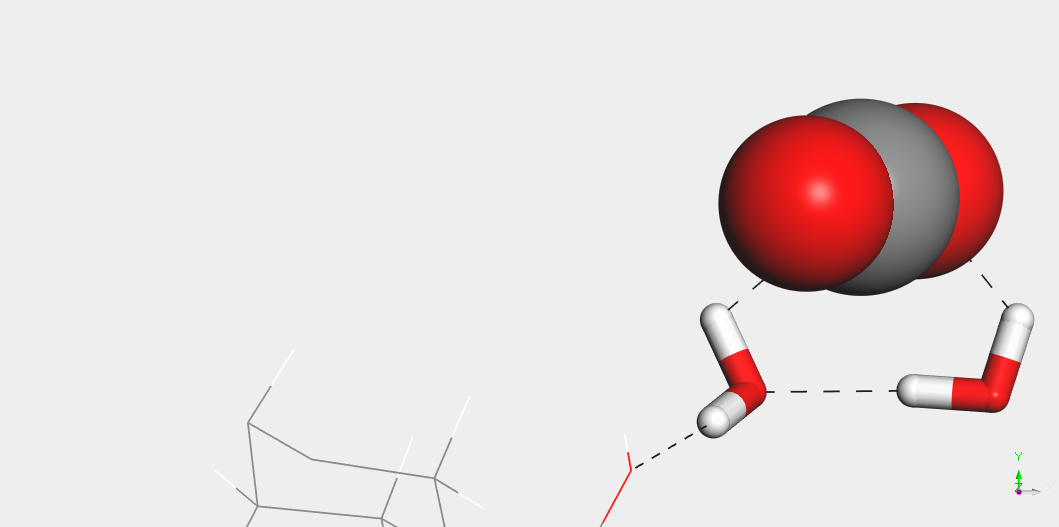
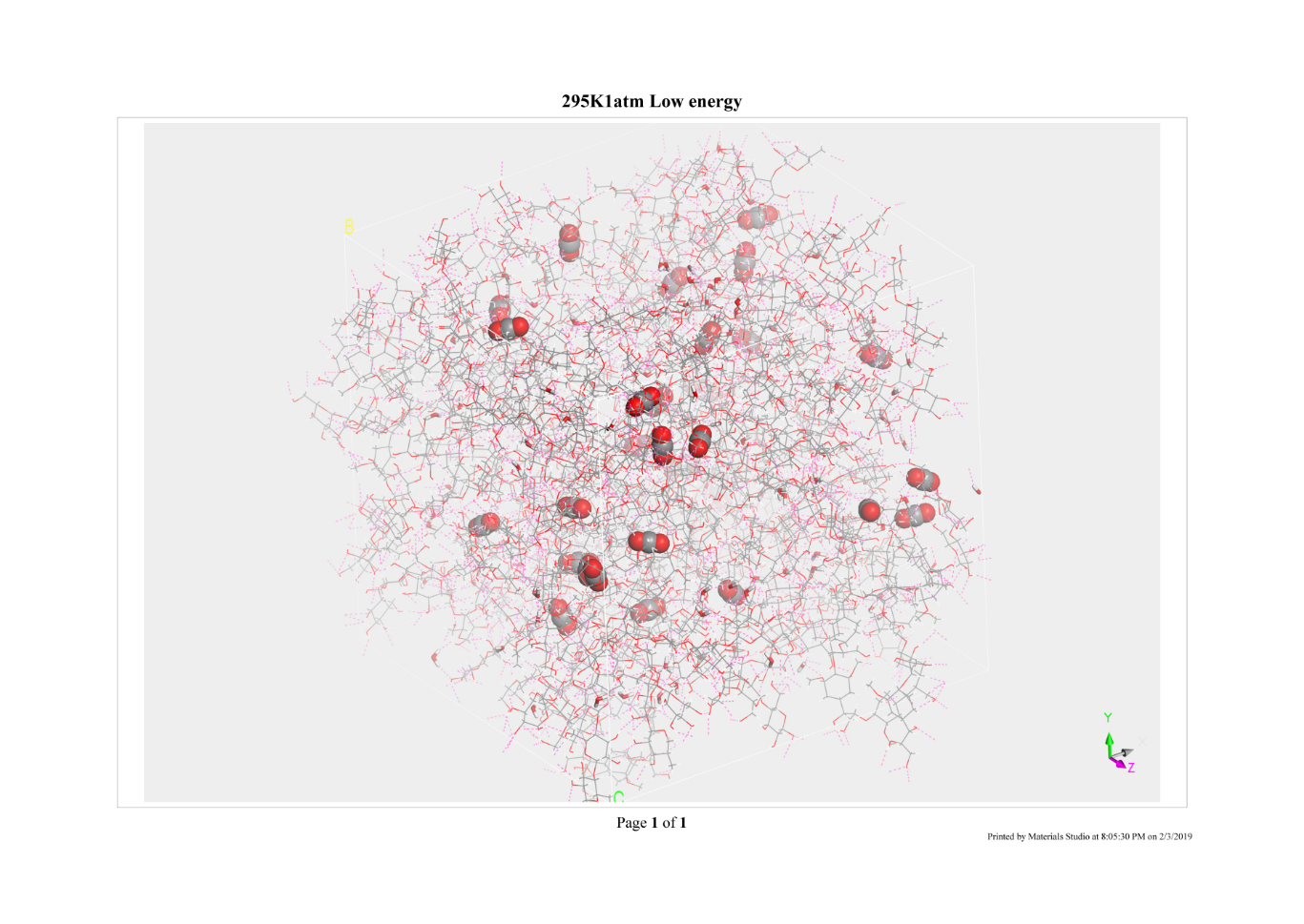


Fig.2. network of interactions among CO2-water-biomass showing CO-OH interaction in CO2-water and HO-H interaction in biomass-water represented by dashed black lines: CO2 in CP2K style, water in stick style, biomass in line style. We suggest these networks as the underlying interplay of water, CO2 and biomass in CO2 uptake and capture by biomass.

The ‘CO2–water-biomass’ network of interactions sharing common water molecule causes that CO2 molecules experience less random movements (mobility) within biomass microstructure in presence of water molecules. In other words, CO2 molecules find less chance to leave moist biomass. Our results show that the mobility of CO2 molecules in presence of water molecules is lower/limited and CO2 molecules experience a much stickier environment and therefore tend to reside in their locations. Our calculated mobility of CO2 in moist biomass is reported in terms of the mean square displacement data as shown in Fig. 3 over a 75 *ps* long simulation averaged over all biomass models. We calculated the diffusivity (*D*) of CO2 within the wet biomass model using the slop of linear correlation to data shown in Fig. 3 as *D* = 0.0214 *A*°2/*ps* (square of Angstrom per Pico second) or 2.14 × 10-6 cm2/s ([Dassault Systemes Materials Studio Tutorials, 2017](#_ENREF_18); [Meunier, 2005](#_ENREF_49)). Thus, wet biomass is able to keep CO2 more reliably. This in turn implies a reliable storage ability/capability, which is highly important when aiming to capture and store CO2 for longer times.

Fig.3. mean square displacement data over 75 ps simulation time (bold solid line) to show low/negligible mobility of CO2 in wet biomass due to the established network of interactions among CO2-water-biomass (averaged over all biomass models). Dashed line shows a linear correlation given as y = 0.1286x + 4.1397. We calculated the diffusivity (*D*) of CO2 within the wet biomass model using this correlation as *D* = 2.14 × 10-6 cm2/s.

Our observation of ‘CO2–water-biomass’ network of interactions sharing common water molecule suggests that moisture alteration can be used as a regulator for CO2 admission in biomass. This brings yet simple but advanced and efficient way for CO2 uptake and release on demand giving the opportunity to design a low cost and sustainable CO2 capture technology. For such freely available resource, biomass brings us a great opportunity to address the global challenge environmental concerns on industrial activities related emissions reduction ([Jacobson, 2009](#_ENREF_31)). In line with the long run researches of adsorptive CO2 capture and storage materials, the slightly moist biomass can be proposed as an excellent adsorbent, the capacity of which can be regulated simply by moisture alteration. Especially as it has been reported that approximately a hundred of water molecules may evaporate from a moist media due to a temperature rise of only one Celsius ([Shusen Wang, 2008](#_ENREF_58)). Such amount of water molecules even can be easily removed or adsorbed through surface evapotranspiration ([Thompson, Benscoter, & Waddington, 2014](#_ENREF_57)). The higher surface temperatures, higher surface evapotranspiration and vice versa ([K. Zhang, Kimball, Nemani, & Running, 2010](#_ENREF_63)). We can conclude the competitiveness of biomass for CO2 capture and storage.

#### Conclusion

Through a number of computational experiments, we were able to examine the potential of biomass for carbon dioxide uptake at ambient conditions. We demonstrated both capture capacity analysis and the mechanism of CO2 adsorption in biomass at ambient conditions. Our simulations showed that the transfer of CO2 molecules into biomass is considerable. We concluded that the biomass CO2 adsorption is governed by ‘CO2–water-biomass’ network of interactions. These networks share same water molecules. The water–CO2 interactions are through CO–OH and the same water molecule participates in water–biomass interaction through H–OH or HO–H. We concluded that CO2 admission into biomass can be regulated and controlled by moisture content. This readily reads that by altering moisture, an efficient and cheap procedure for CO2 uptake and release on demand is achievable. Biomass gives the opportunity to design a low cost and sustainable CO2 capture technology with a capacity around 50 gr CO2/gr biomass.

**Conflict of interest**

There is no conflict of interest.

Data availability

The article has associated supplementary files which are available both at the publisher website and can be requested from the authors at:

<https://sites.google.com/site/miladasgarpour/Posts/Completed/CO2Biomass>.

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