Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary data

1.Image analysis of high resolution transmission electron micrographs (HRTEM)

A semi-automated procedure in Adobe Photoshop coupled with Matlab was applied to extract parameters regarding fringe width, orientation angles and centroid coordinates from HRTEM images. This processing procedure derived from Enette [1], includes following steps of (1)contrast enhancement, (2)histogram equalization, (3)Gaussian blur, (4)fast Fourier transform filtering, (5)band-pass filtering, (6)smooth filtering, (7)inverse Fourier transform filtering, (8)binary image conversion, and (9)skeletonization, as shown in Figure 1. Finally, fringes smaller than 3Å were rejected, since they could be considered as noise and removed without loss of data [2-5].

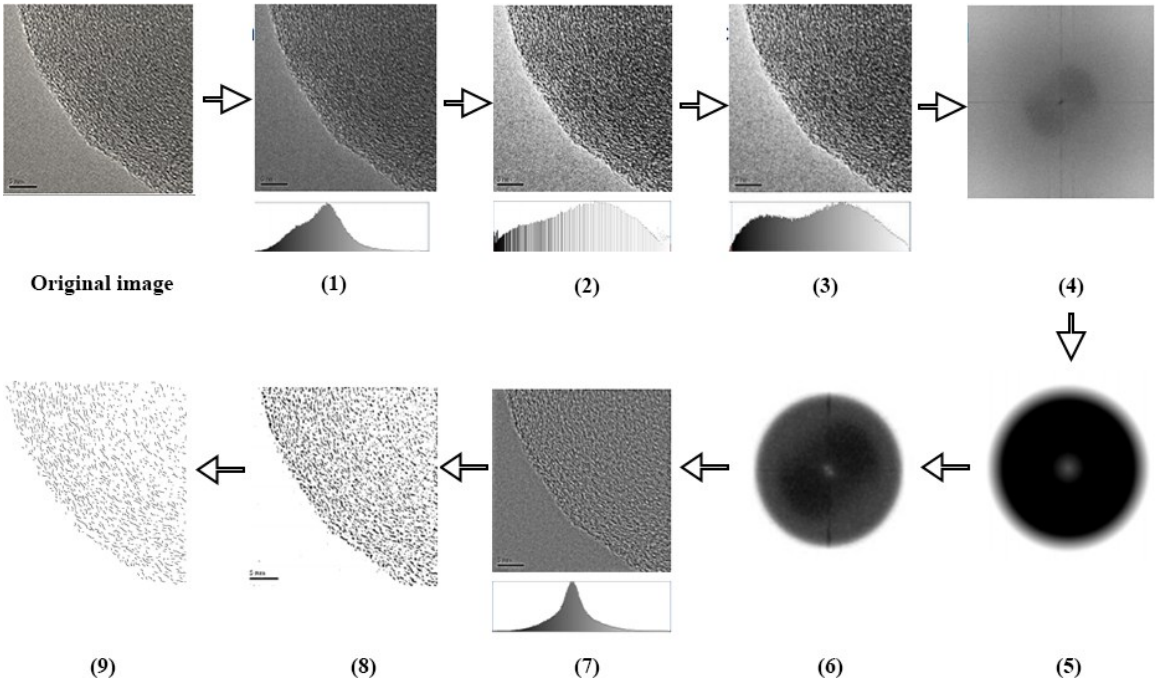


Fig.1 The processing procedure of HRTEM image analysis

The extract parameters, including skeleton length, centroid coordinates and moment angle are interpreted in Matlab, where a graphical user interface (GUI) are developed to identify stack distributions [1]. Herein, the authors set the parameter of midpoint distance (7.0Å), perpendicular distance (4.0Å) and angle difference (30°), as demonstrates in Figure 2. The program compared the information of one fringe relative to all other fringes, and if all three of these conditions were met, fringe characterizations were identified as part of a multiple fringe stack. A final check was conducted to ensure no fringe formed a part of more than one recognized stack.

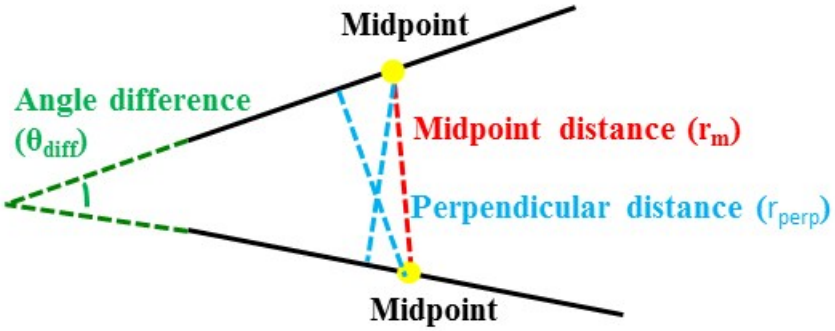


Fig.2 Illustration of distance between fringe midpoints and perpendicular distances between two fringes

2. Experimental characterization of lignite-based activated carbon

The lignite-based activated carbon used in this research originated from Norit Americas Inc, identified as SuperDarco. Prior to tests, the samples were crushed and sieved to 200×400 US mesh size. Experimental characterization included mercury porosimetry, helium picnometry, elemental analysis, pore size distribution and Brunauer-Emmett-Teller surface area. Testing methods and results were shown in Table1.

Table 1 Analytical Characterization of lignite-feed activated carbon identified as "SuperDarco"

Characterization	Experimental Values	Instruments and/or methods
Pore volume distribution (Nitrogen)		ASAP 2020
Micropores (< 20Å)	0.252 mL/g	(Micromeritics, USA)
Mesopores (20~310Å)	0.506 mL/g	
Large Mesopores (310~500Å)	0.041 mL/g	
Surface area	879 m²/g	Brunauer-Emmett-Teller method
Apparent density	0.33 g/ml	Packed-bed dry density
Mercury porosimetry		Autopore IV
2,000,000~490,000Å	0.120 mL/g	(Micromeritics, USA)
490,000~310Å	1.848 mL/g	
310~36Å	0.489 mL/g	
Helium picnometry	2.20 g/mL	AccuPyc 1330 Pycnometer (Micromeritics, USA)
Ash content	16.93%	ASTM Designation: D3174 − 12

Elemental composition, atomic %		2400 Series II CHNS/O System
Carbon	68.52%	(PerkinElmer, USA)
Hydrogen	12.04%	
Oxygen	19.16%	
Nitrogen	0.28%	

The adsorption isotherm of nitrogen at 77K exhibited a combination of Type I and IV profile according to IUPAC classification was shown in Figure 3. A sharp uptake at low relative pressure indicated a microporous structure. The initial part of the curve was attributed to monolayer-multilayer adsorption, whereas the hysteresis loop was associated with capillary condensation taking place in the mesopores [6]. The lower end of the hysteresis loop approximately occurred at p/p_0=0.4, indicating that the capillary condensation might start from a pore size at about 30Å [7].

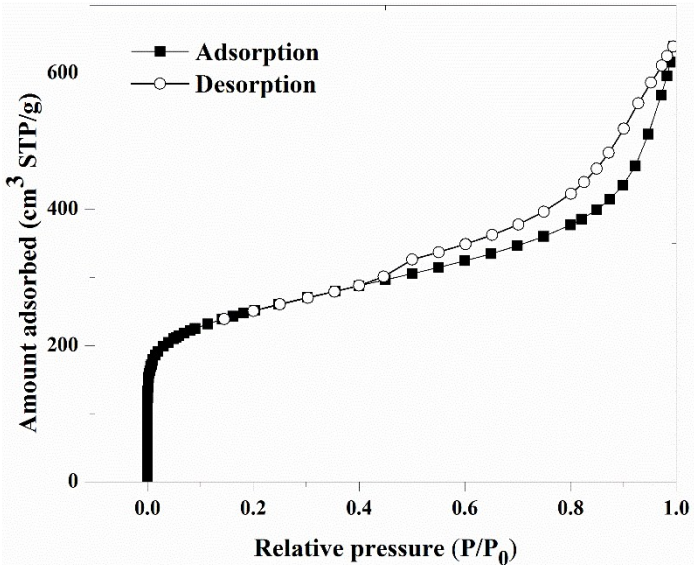
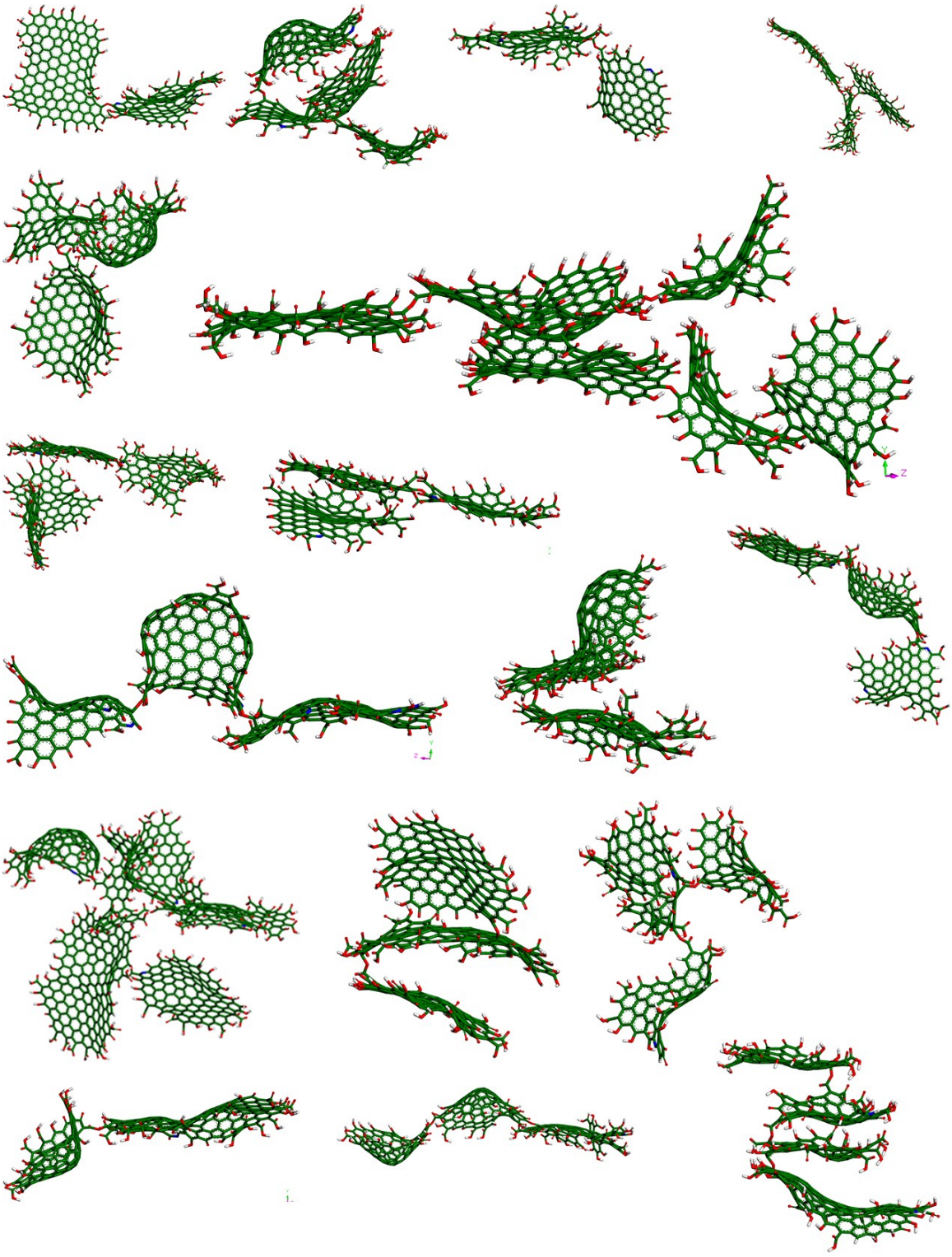
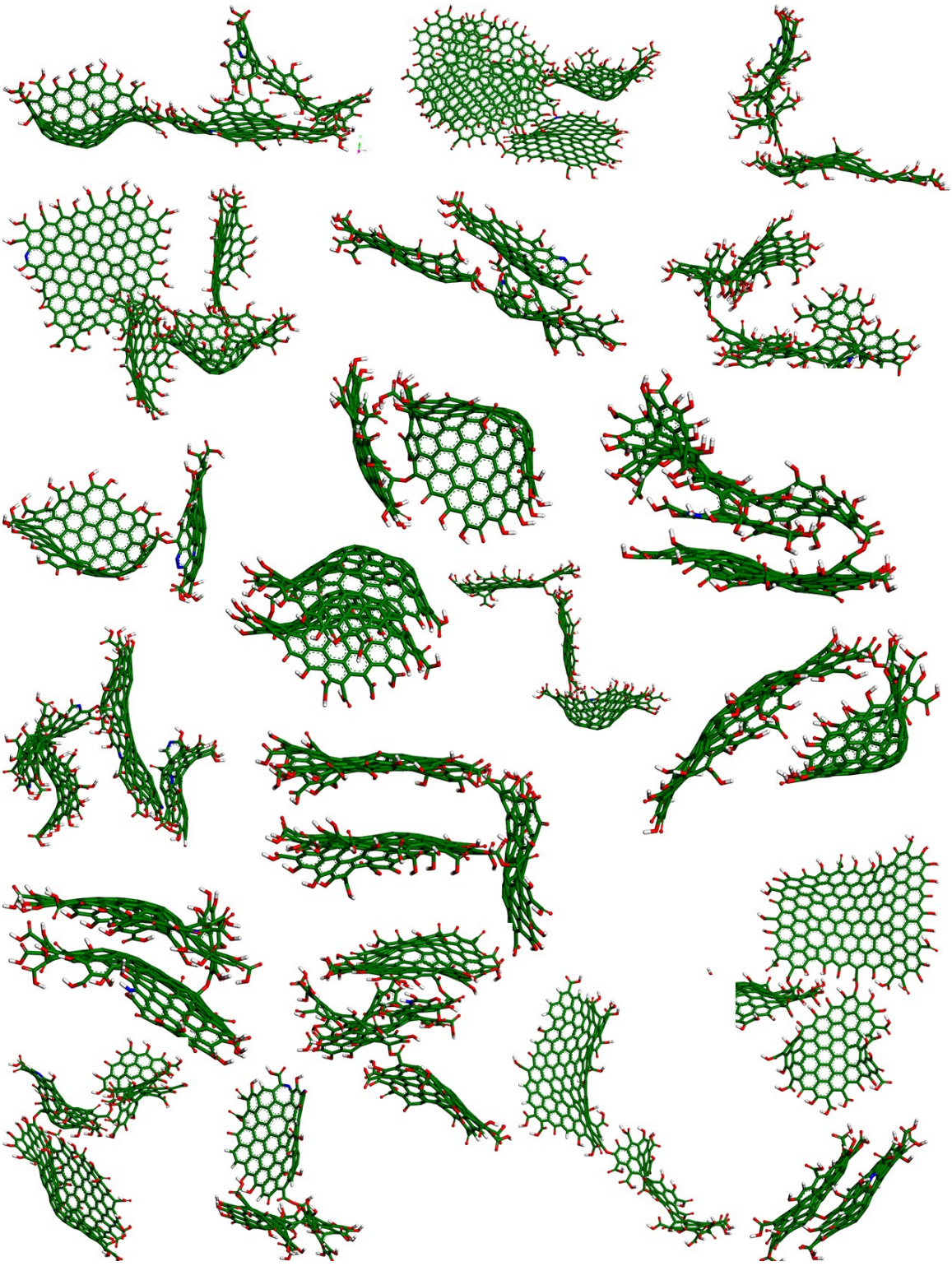


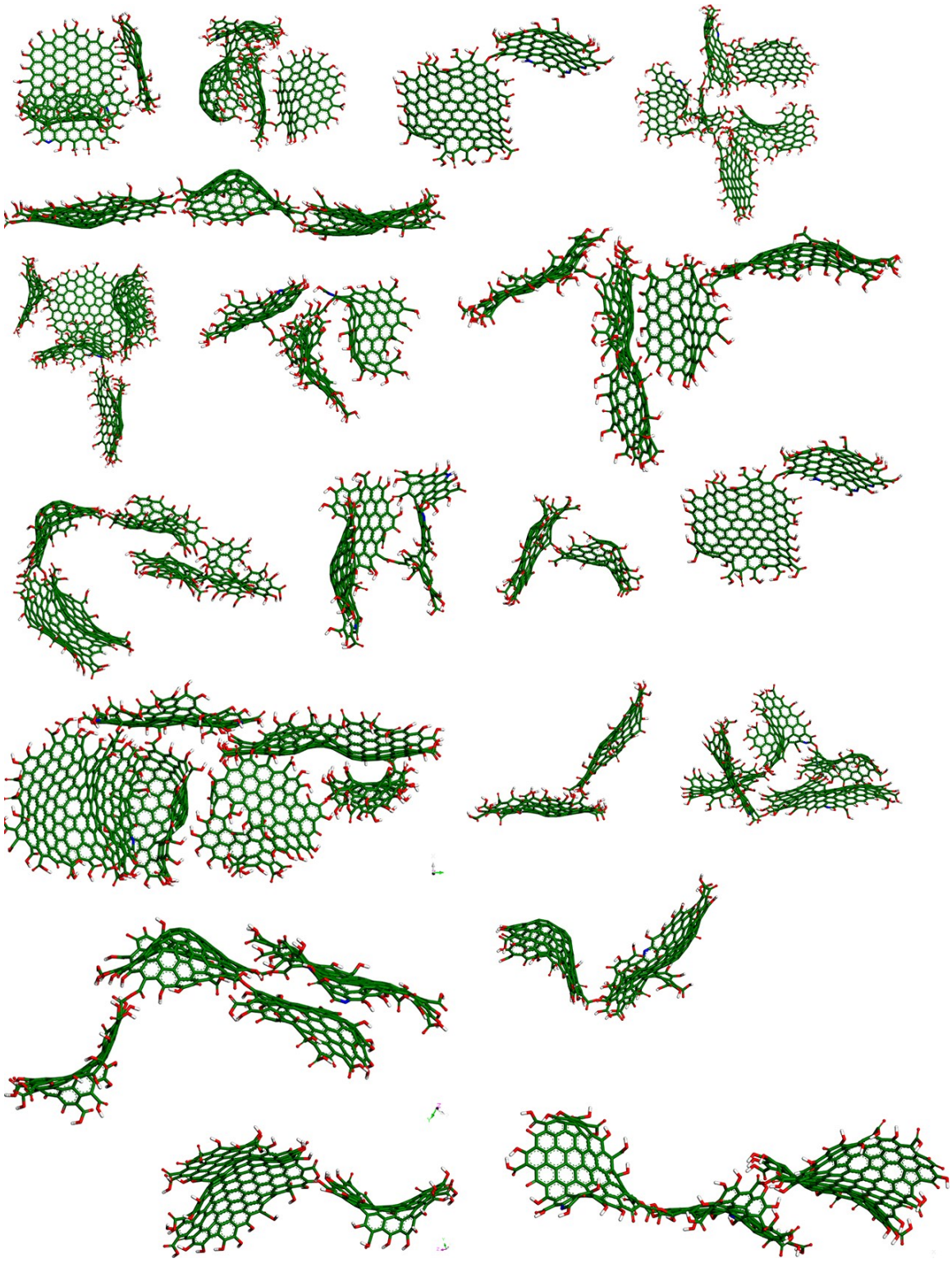
Fig.3 Adsorption and desorption isotherm of nitrogen at 77K

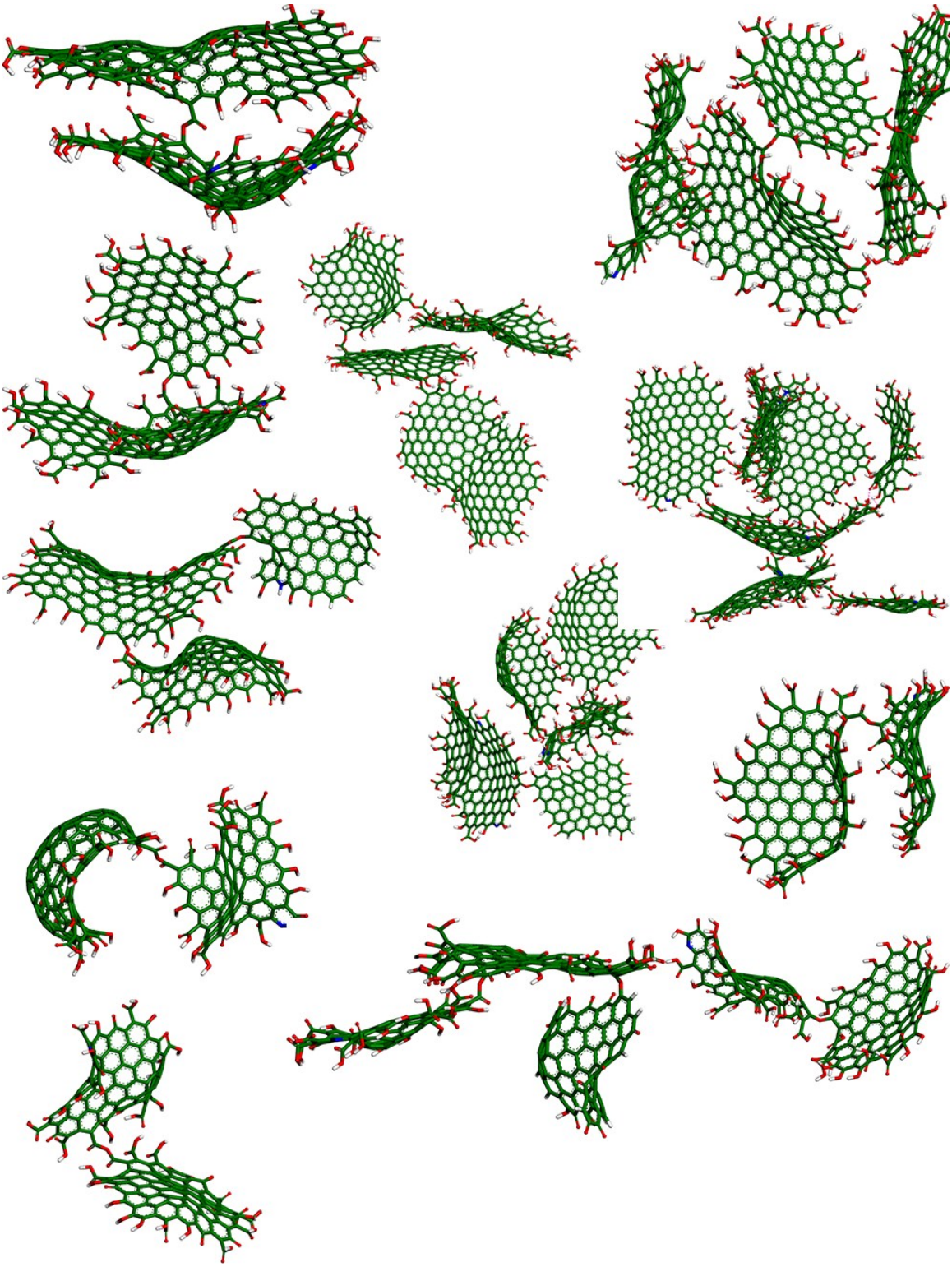
2. Cross-linked clusters in the simulated models





Microporous model 1





Micro/mesoporous model 2

Reference

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4 Sharma A, Kyotani T, Tomita A. A new quantitative approach for microstructural analysis of coal char using HRTEM images. Fuel. 1999;78(10):1203-12.

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