Supplementary Information

Combined experimental and molecular simulation study on H_2 storage in oxygen and nitrogen co-doped activated carbon derived from biomass waste: Superior pore size and surface chemistry development

by

Suphakorn Anuchitsakol,[a] Waralee Dilokekunakul,[b] Numphueng Khongtor,[c] Somboon Chaemchuen,[d] Nikom Klomkliang *[a,e]

[a] School of Chemical Engineering, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

[b] Aachener Verfahrenstechnik - Chemical Process Engineering, RWTH Aachen University, Aachen 52074, Germany

[c] Institute of Research and Development, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

[d] State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China.

[e] Research Unit of Adsorption, Catalysis & Energy Storage, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

* Corresponding author: E-mail address: nikom.klo@sut.ac.th

Table S1. Molecular parameters for H_2 and functional groups used in this work.

Fluid/Functional group	**ε/k_B (K)**	**σ (nm)**	**q (e)**
H_2			
H	-	-	+0.4829
Center of mass	36.500	0.282	−0.9658
Hydroxyl			
C	28.000	0.340	+0.2000
O	78.994	0.310	−0.6400
H	30.000	0.131	+0.4400
Carbonyl			
O	78.994	0.310	−0.5000
C	28.000	0.340	+0.5000
Carboxyl			
C	28.000	0.340	+0.5500
O (=O)	78.994	0.310	−0.5000
O (-O-)	78.994	0.310	−0.5800
H	30.000	0.131	+0.4500
Pyrrolic-N			
C (CN)	28.000	0.340	+0.31
N	60.388	0.3296	−0.96
H (NH)	30.000	0.131	+0.46
Pyridinic-N oxide			
C (CN)	28.000	0.340	+0.34
N	60.388	0.3296	−0.52
O (NO)	78.994	0.31	−0.47
Quaternary-N			
C (CN)	28.000	0.340	+0.37
N	60.388	0.3296	−1.17

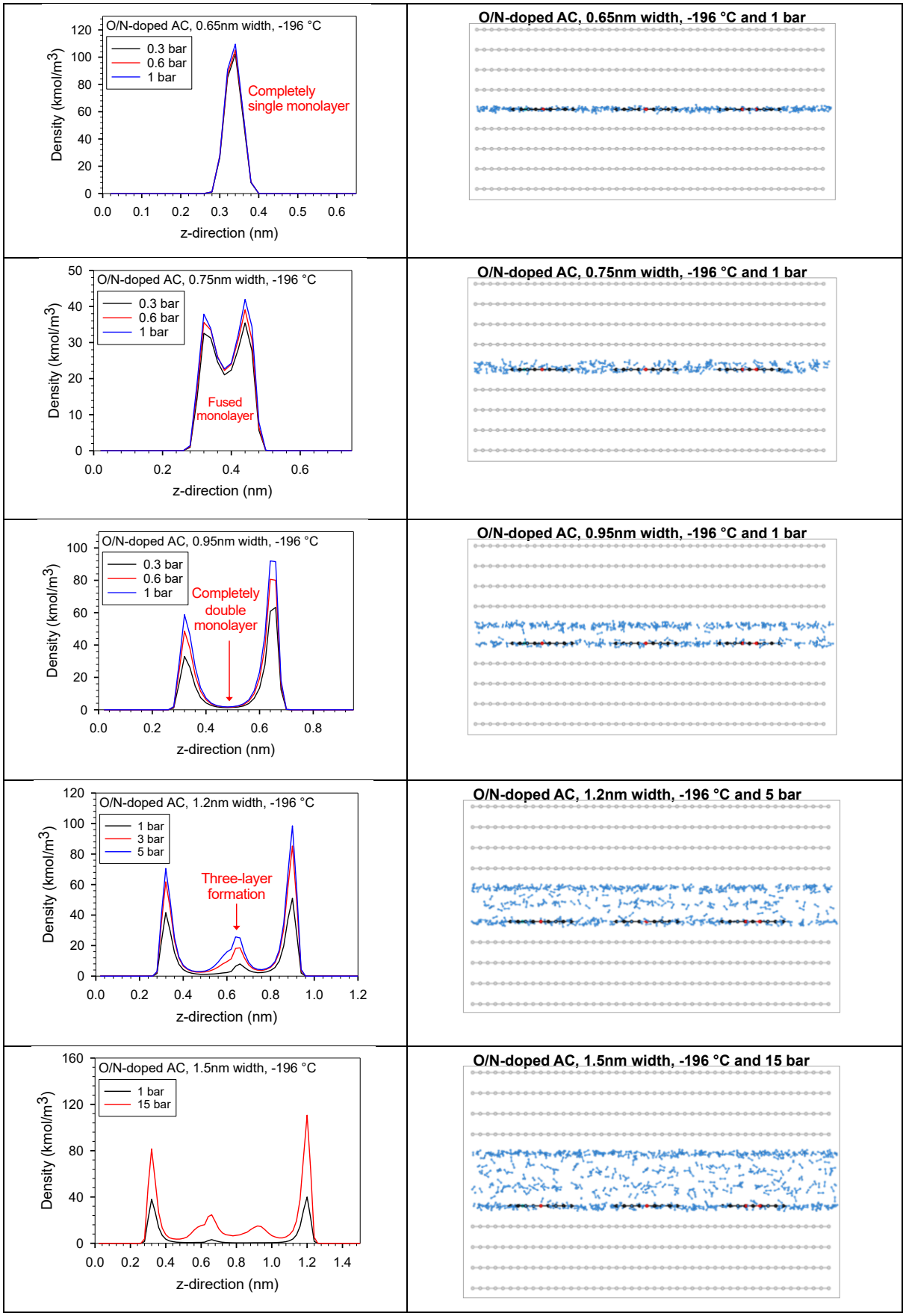

Figure S1. Local density distributions and snapshots of H_2 on various pore widths and pressures at −196°C.

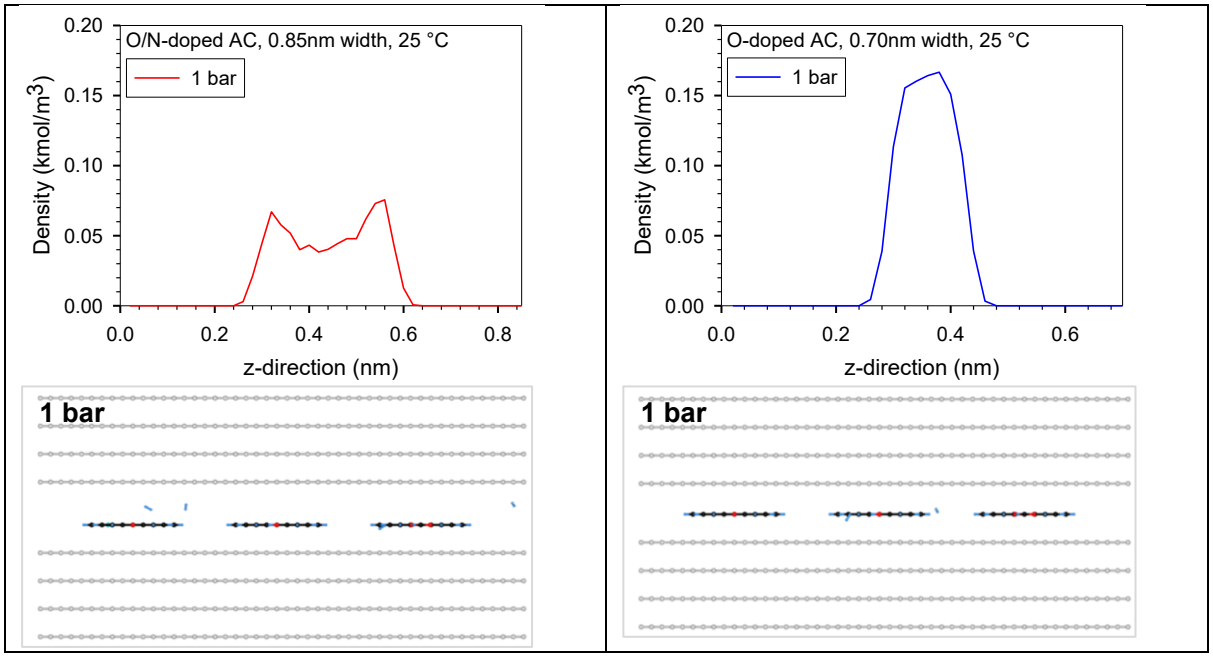

Figure S2. Local density distributions and snapshots of H_2 adsorption in O/N-doped AC model (0.85 nm width) and O-doped AC model (0.70 nm width) at 25ºC.

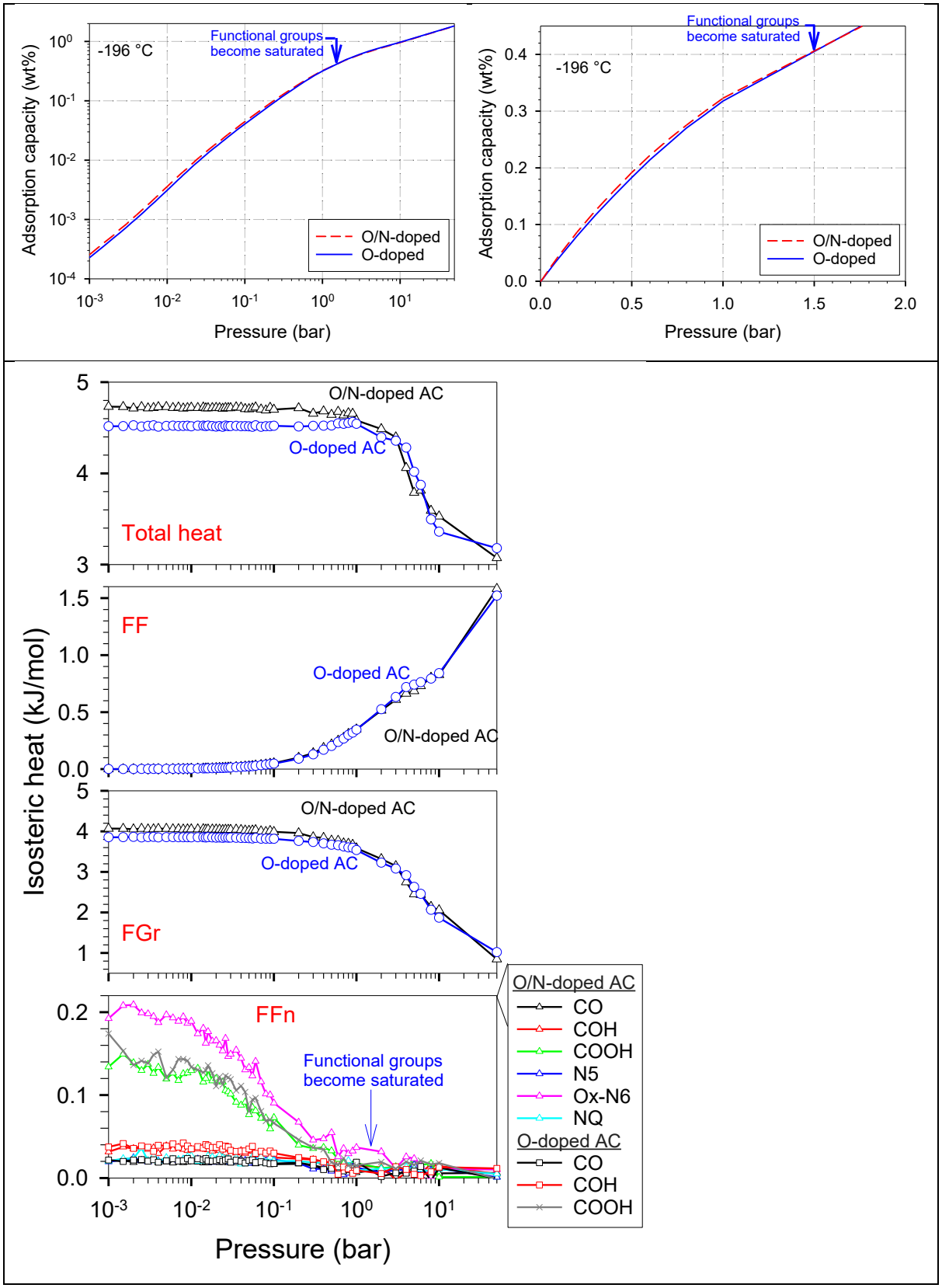

Figure S3. Isotherms and isosteric heats of H_2 adsorption in O/N-doped AC model and O-doped AC model at −196ºC obtained with GCMC.