Supporting Information

Molecular Modeling and Adsorption Properties of Ordered Silica Templated CMK Mesoporous Carbons

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This supporting information includes

1. Schematic of simulation methodology of obtaining CMK models
2. Argon adsorption isotherms for CMK-1 models and experimental nitrogen adsorption isotherm for a CMK-1 sample
3. Isosteric heat of adsorption of CMK-1, CMK-3 and CMK-5 models
4. Framework densities of CMK models

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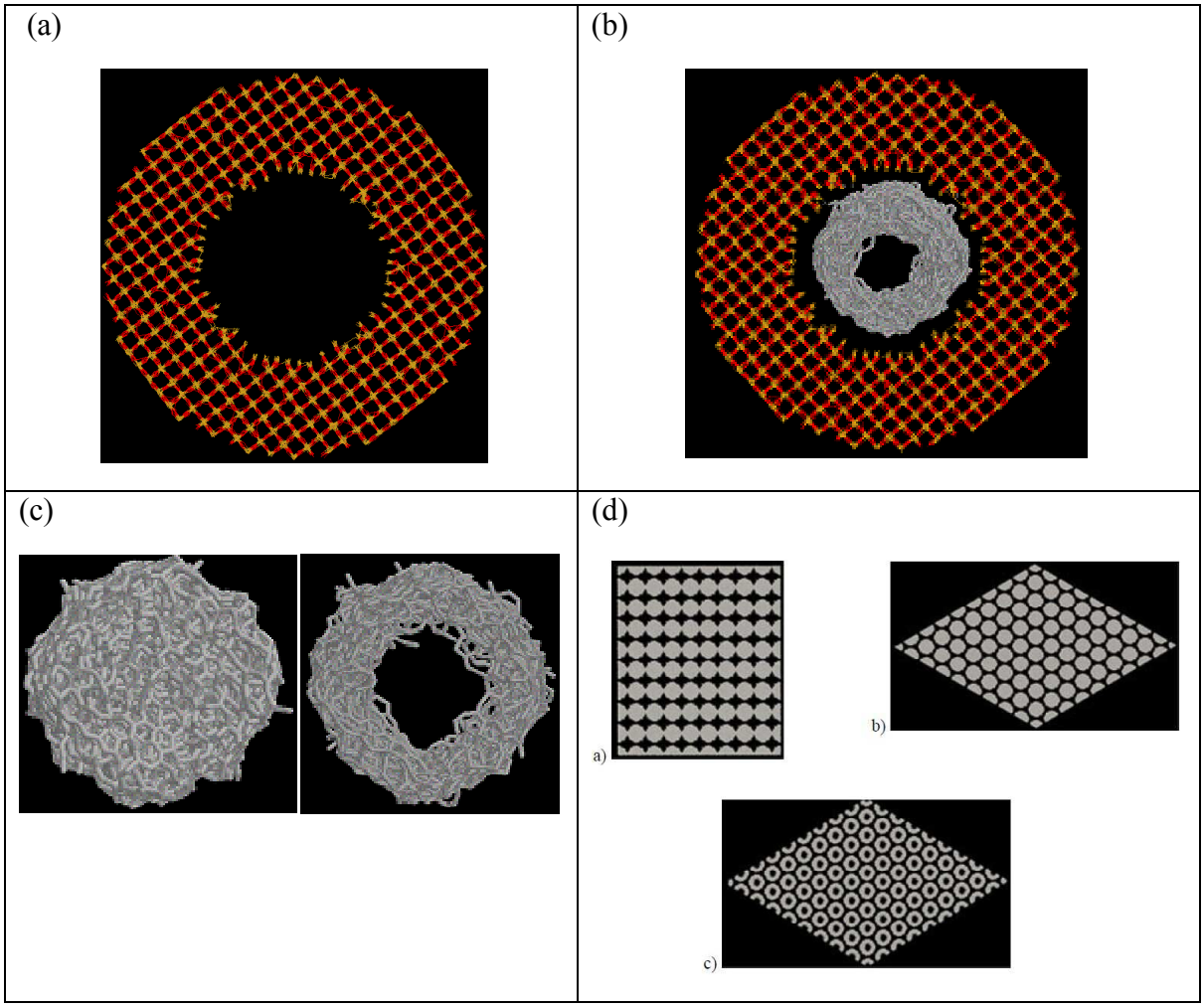

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Figure S1: *Schematic showing the simulation methodology of obtaining CMK models from MCM-41 pore (a)MCM-41 pore, (b) Carbon adsorption inside MCM-41 pore to obtain carbon rods and carbon pipes (c) Removal of silica template and relaxation of carbon pipes and rods (d) Arrangement of carbon rods in cubical lattice to get CMK-1 model, arrangement of carbon rods in hexagonal lattice to get CMK-3 model and arrangement of carbon pipes in hexagonal lattice to get CMK-5 model*

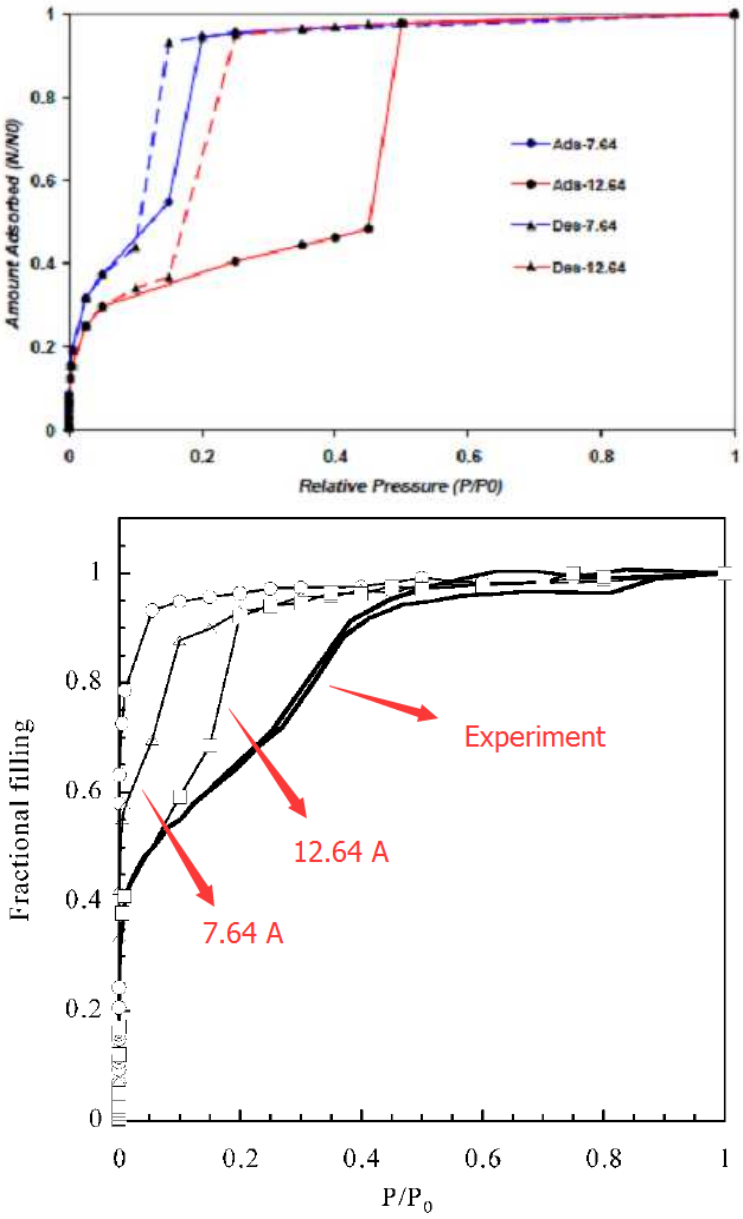

Figure S2: *Argon adsorption isotherms at 77 K in CMK-1 models (top) and the nitrogen adsorption isotherms obtained at 77 K from RSP model and experiment [7] (bottom).*

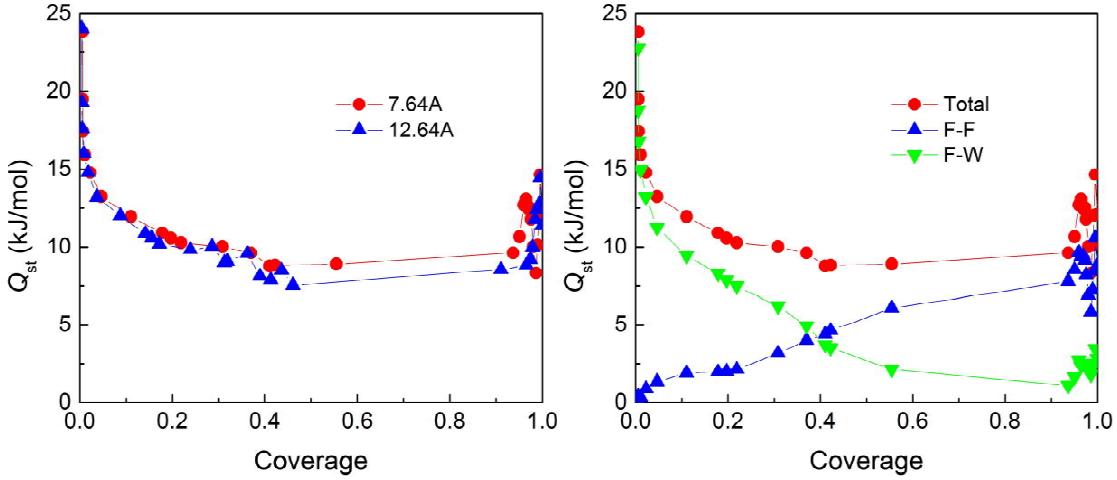

Figure S3: *Isosteric heat of adsorption of CMK-1 models for 7.64A and 12.64A pore width (left). Total, Fluid-Fluid and Fluid-Wall contribution to 7.64A pore width (right)*

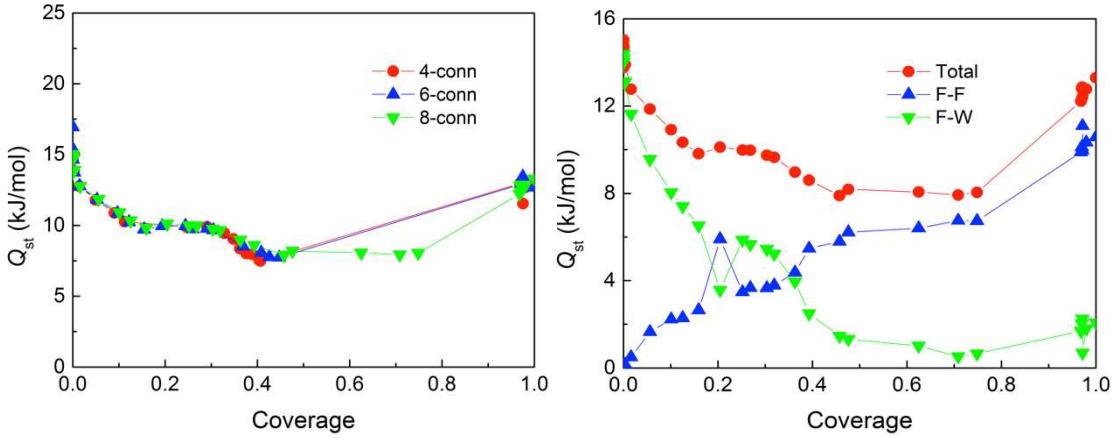

Figure S4: *Isosteric heat of adsorption for the CMK-5 models with interconnections (left) and the total, fluid-fluid, fluid-wall contributions to the isosteric heat of CMK-5 model with 8 interconnections.*

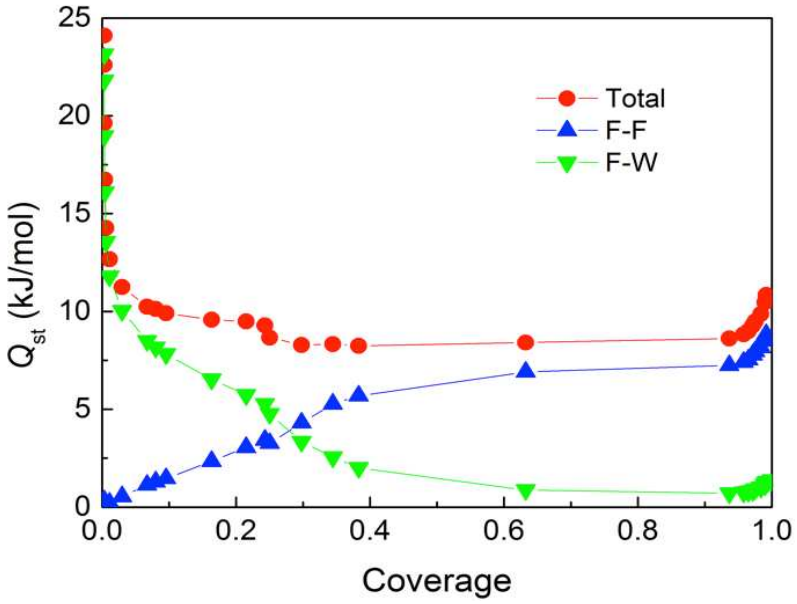

Figure S5: *Isosteric heat of adsorption for the CMK-3 models with 8 interconnections. Total, fluid-fluid, fluid-wall contributions to the isosteric heat.*

Table S1: *Calculated framework density of CMK materials*

Materials	ρ_f (g/cm^3)
CMK-1, 7.64A	1.108
CMK-1, 12.64A	0.978
CMK-3, 14A-8c	0.841
CMK-5, 14A-8c	0.439