

Supporting information for

Role of Porosity and Polarity of Nanoporous Carbon Spheres in Adsorption Applications

Hee Soo Kim¹, Seunghun Lee¹, Dong Kwan Kim¹, Yong-Woo Lee^{1,2,*}, and Won Cheol Yoo^{1,2,*}

¹ Department of Applied Chemistry, Hanyang University, Ansan 15588, Republic of Korea
E-mail: yongwoolee@hanyang.ac.kr; E-mail: wcyoo@hanyang.ac.kr

² Department of Chemical and Molecular Engineering, Hanyang University, Ansan 15588,
Republic of Korea

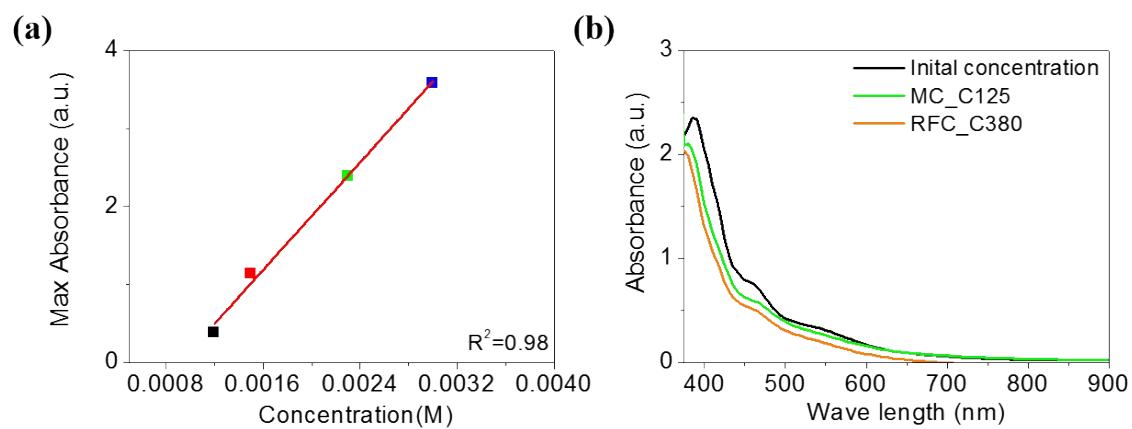


Fig S1. The calibration curve of the different concentrations of Fe^{2+} (a) and UV-Vis results for carbon samples (b).

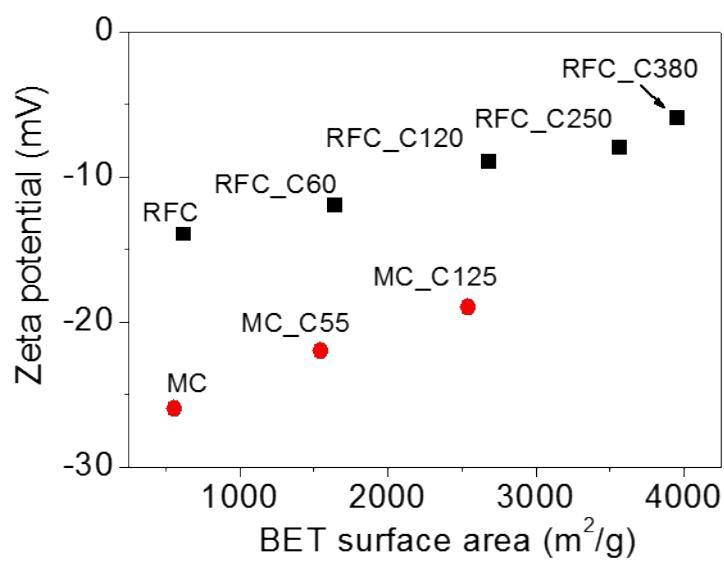


Fig S2. The zeta potential results for RFC and MC samples

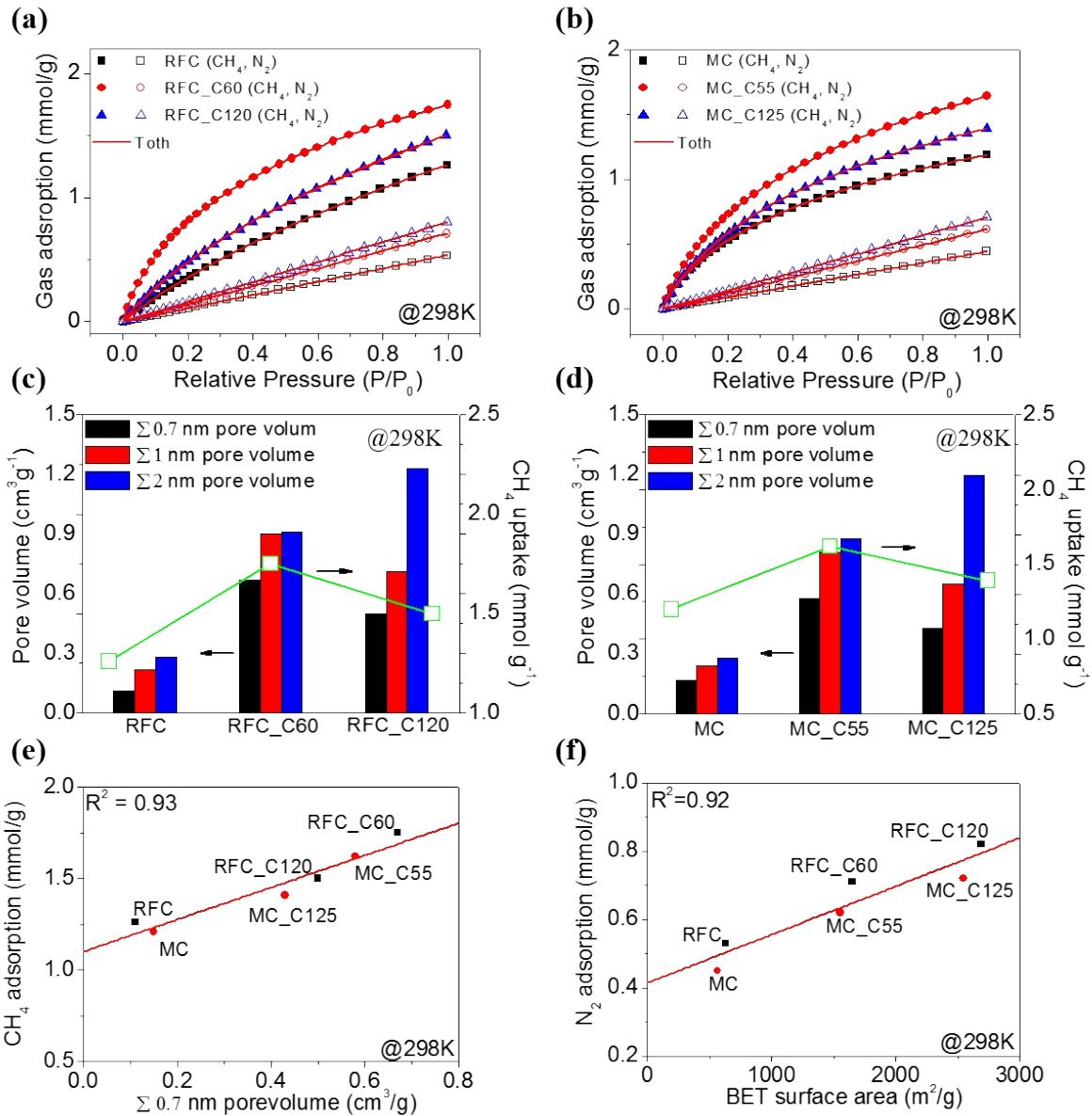


Fig S3. CH_4 and N_2 isotherm of RFC (a) and MC (b) samples at 298K (red line is Toth isotherm fitting). Distribution of pore volumes between pores of less than 0.7 nm (black), less than 1 nm (red), and less than 2 nm (blue) of RFC (c) and MC (d) samples at 298K. Relationship plot of CH_4 adsorption capacities with respect to accumulated ultramicropore volume of 0.7 nm (e) and Relationship plot of N_2 adsorption capacities with respect to BET surface area (d) of RFC and MC samples at 298K

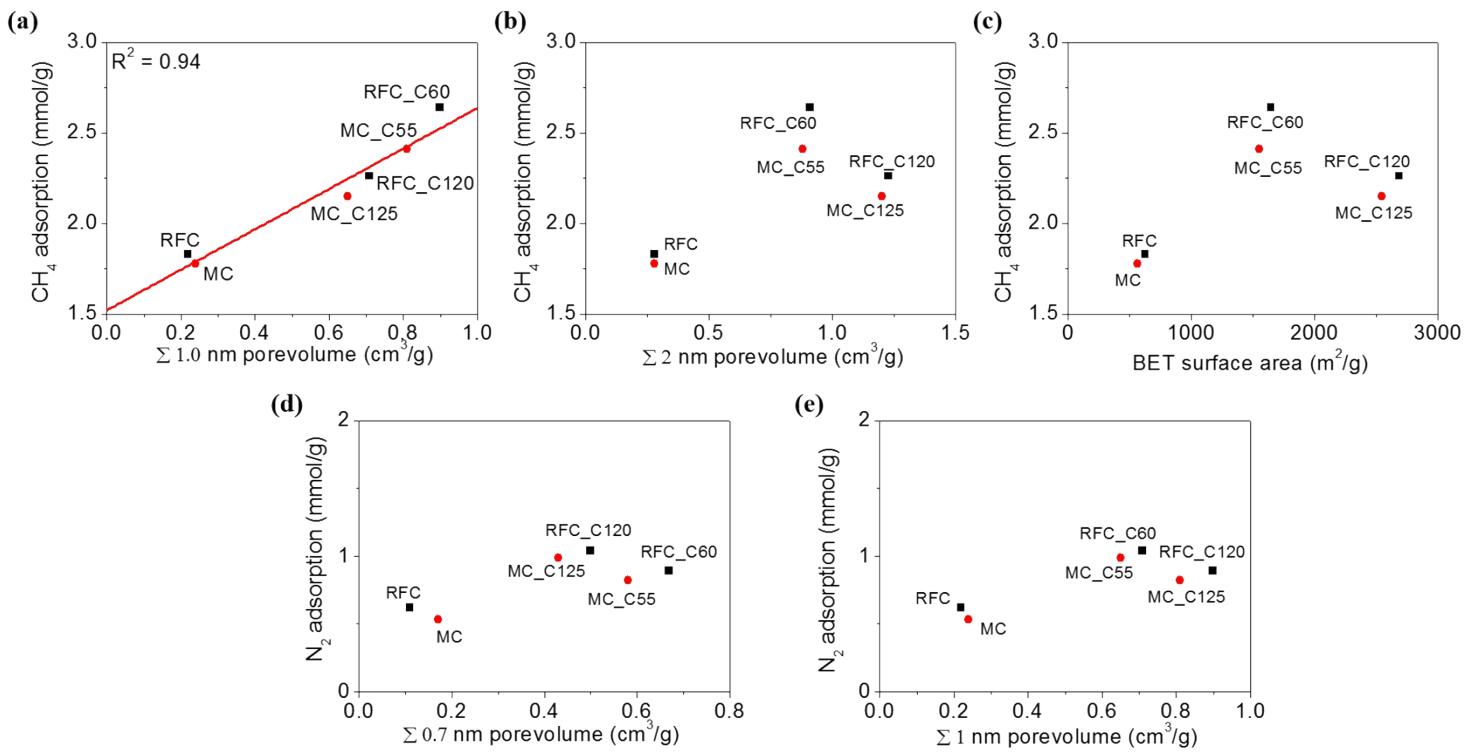


Fig S4. Relationship plot of CH₄ adsorption capacities with respect to accumulated ultramicropore volume of 1 nm (a), 2 nm (b) and BET surface area (c) of RFC and MC samples at 273K. Relationship plot of N₂ adsorption capacities with respect to accumulated ultramicropore volume of 0.7 nm (d) and 1 nm (e) of RFC and MC samples at 273K.

| Wavenumber (cm ⁻¹) | Functional group |
|--------------------------------|---|
| 1260 | Pyrrole ring out of plane |
| 1389 | C-N stretching |
| 1405 | Pyridine N oxide (N=O vibrations) |
| 1513 | C=N vibrations |
| 1610 | COO antisymmetric stretch / C=C aromatic ring vibration |

Table S1. Assignments of FT-IR peaks of RFC_C60 and MC_C55.

| Sample | q_m / CH_4 (273K / 298K) | q_m / N_2 (273K / 298K) | K_i / CH_4 (273K / 298K) | K_i / N_2 (273K / 298K) | n / CH_4 (273K / 298K) | n / N_2 (273K / 298K) |
|----------|--------------------------------------|-------------------------------------|--------------------------------------|-------------------------------------|------------------------------------|-----------------------------------|
| RFC | 2.6 / 2.34 | 1.4 / 1.1 | 1.12 / 0.74 | 0.51 / 0.36 | 0.67 / 0.63 | 0.91 / 0.95 |
| RFC_C60 | 3.2 / 2.84 | 1.6 / 1.3 | 1.4 / 0.98 | 0.55 / 0.4 | 0.5 / 0.52 | 0.88 / 0.89 |
| RFC_C120 | 2.82 / 2.55 | 1.82 / 1.59 | 1.24 / 0.87 | 0.65 / 0.52 | 0.58 / 0.56 | 0.8 / 0.82 |
| MC | 2.51 / 2.12 | 1.0 / 0.91 | 1.02 / 0.7 | 0.45 / 0.3 | 0.68 / 0.65 | 0.92 / 0.94 |
| MC_C55 | 2.9 / 2.41 | 1.2 / 1.0 | 1.31 / 0.94 | 0.47 / 0.32 | 0.51 / 0.54 | 0.9 / 0.92 |
| MC_C125 | 2.75 / 2.26 | 1.67 / 1.54 | 1.11 / 0.79 | 0.57 / 0.5 | 0.6 / 0.58 | 0.81 / 0.84 |

Table S2. Parameters obtained from Töth models for CH₄ and N₂ adsorption at 273K and 298K.

| Sample | CH ₄ Adsorption (273K/298K) (mmol/g) | N ₂ Adsorption (273K/298K) (mmol/g) | CH ₄ Slope (273K/298K) (0-0.1 bar) | N ₂ Slope (273K/298K) (0-0.1bar) | Selectivity (CH ₄ /N ₂) (273K/298K) |
|----------|--|---|--|--|--|
| RFC | 1.83 / 1.26 | 0.62 / 0.53 | 4.0 / 2.1 | 1.05 / 0.51 | 3.8 / 4.2 |
| RFC_C60 | 2.64 / 1.75 | 0.89 / 0.71 | 5.8 / 4.9 | 1.01 / 0.72 | 5.7 / 6.8 |
| RFC_C120 | 2.26 / 1.50 | 1.04 / 0.82 | 4.13 / 3.2 | 0.84 / 0.6 | 4.9 / 5.3 |
| MC | 1.78 / 1.19 | 0.59 / 0.45 | 4.2 / 3.2 | 0.9 / 0.6 | 4.7 / 5.3 |
| MC_C55 | 2.41 / 1.62 | 0.82 / 0.62 | 6.2 / 4.46 | 1.01 / 0.6 | 6.1 / 7.4 |
| MC_C125 | 2.15 / 1.39 | 0.99 / 0.72 | 5.4 / 3.94 | 0.95 / 0.66 | 5.7 / 6.0 |

Table S3. CH₄, N₂ uptake capacities and CH₄, N₂ slope at 0 – 0.1 bar for RFC and MC samples.