

Supporting Information

Aggregation Structure of Polycarbosilane

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The pore volume of micropores with pore widths less than 2 nm were calculated based on the N₂ adsorption-desorption isotherm of PCS2 according to several methods including density functional theory (DFT), non-local density functional theory (NLDFT), Horvath-Kawazoe (H-K), Dubinin-Astakhov (D-A), Dubinin-Radushkevich (D-R), t-plot and MP, respectively. The selected models with hypothesis of pore shapes and the obtained pore volumes were summarized in Table S1.

Table S1. Pore volume of micropores calculated based on different methods with corresponding hypothesis of pore shape

Method	hypothesis of pore shape	Pore volume(cm ³ /g)
DFT	slit	0.0003(6)
NLDFT	slit	0.0005(8)
H-K	slit	0.0014(5)
D-A	slit	0.0019(1)
D-R	/	0.0009(6)
t-plot	/	/
MP	cylinder	0