



Article

# Molecular Investigation of CO<sub>2</sub>/CH<sub>4</sub> Competitive Adsorption and Confinement in Realistic Shale Kerogen

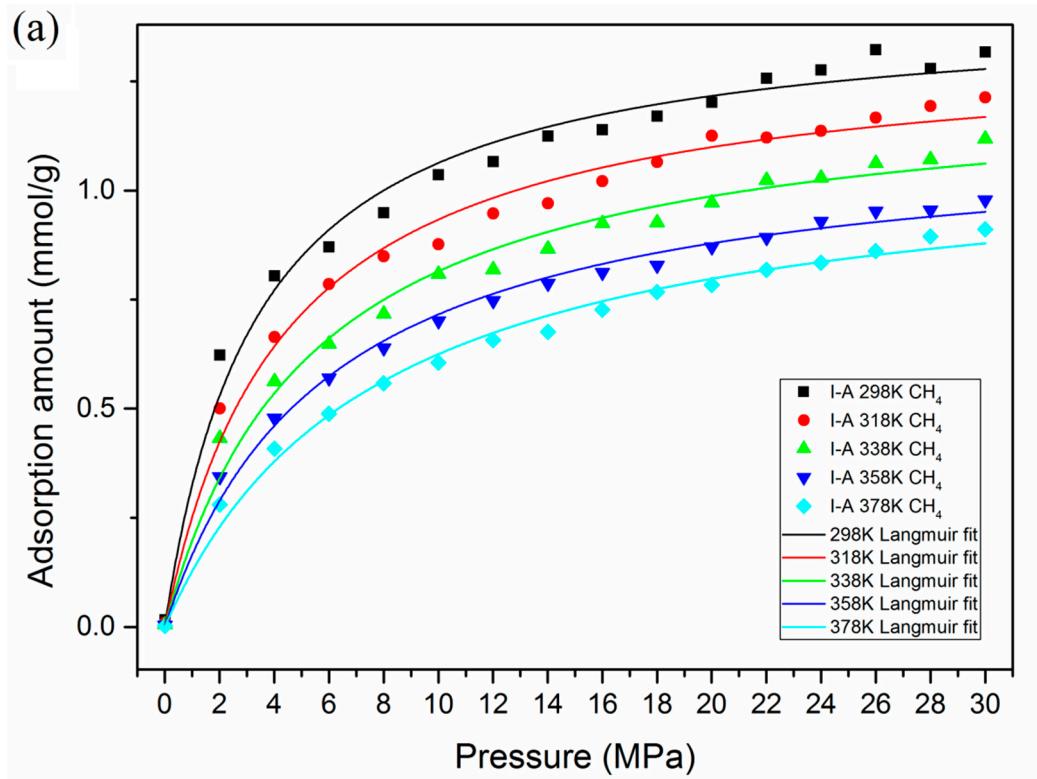
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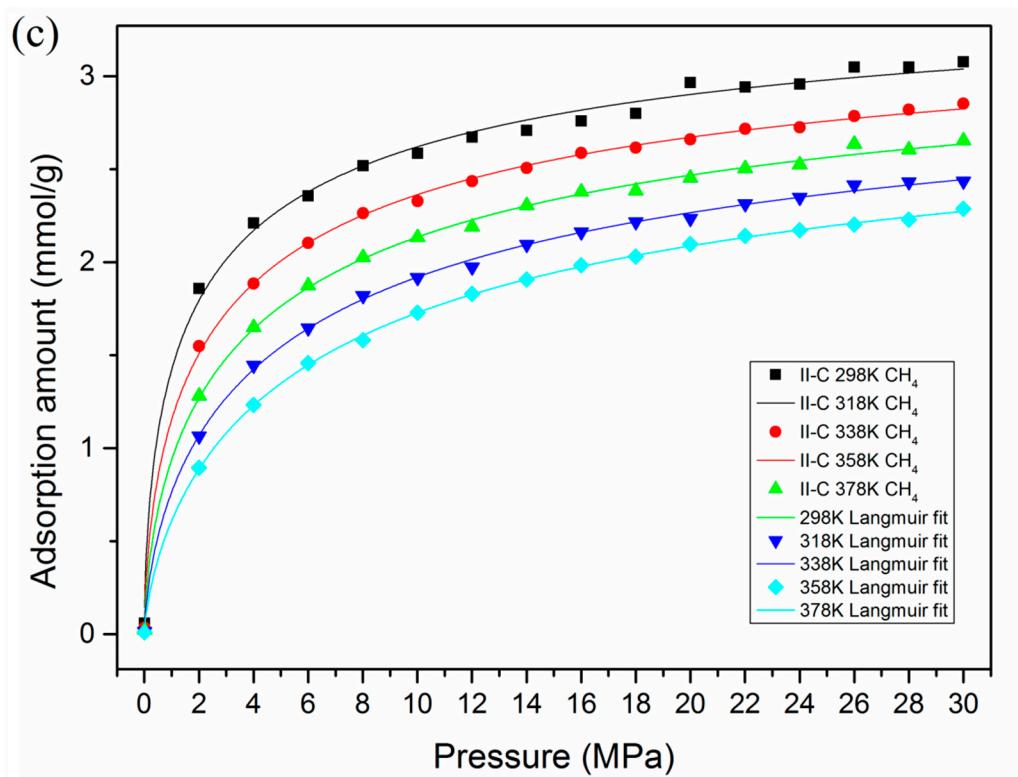
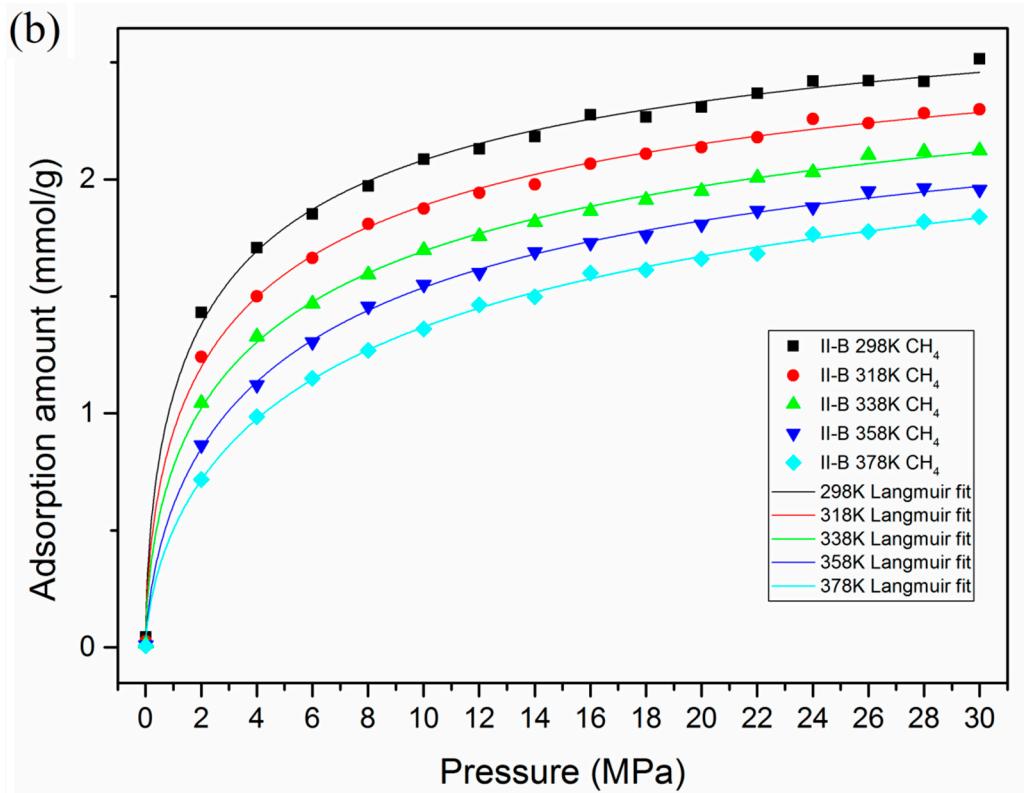
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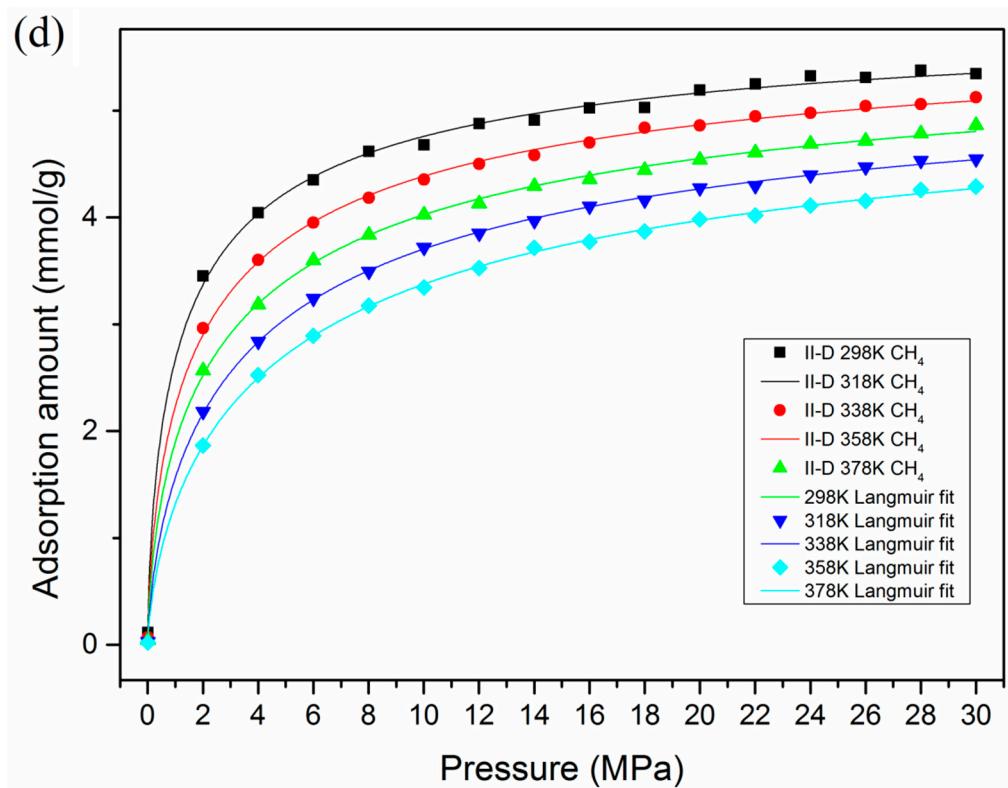
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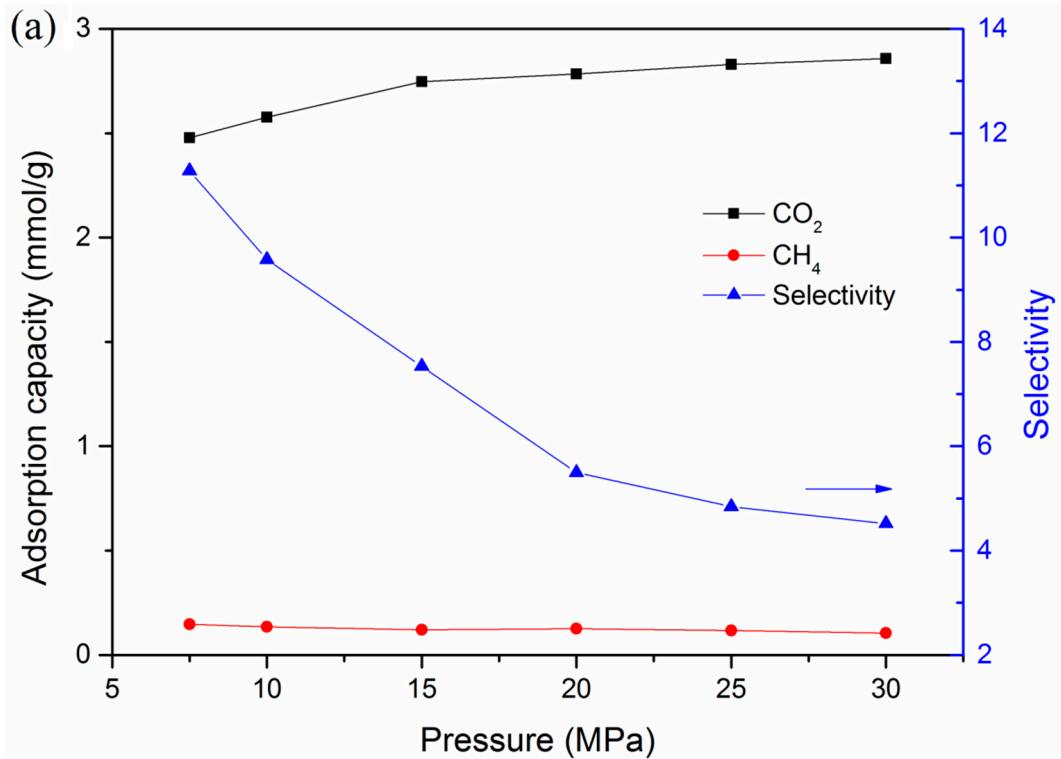
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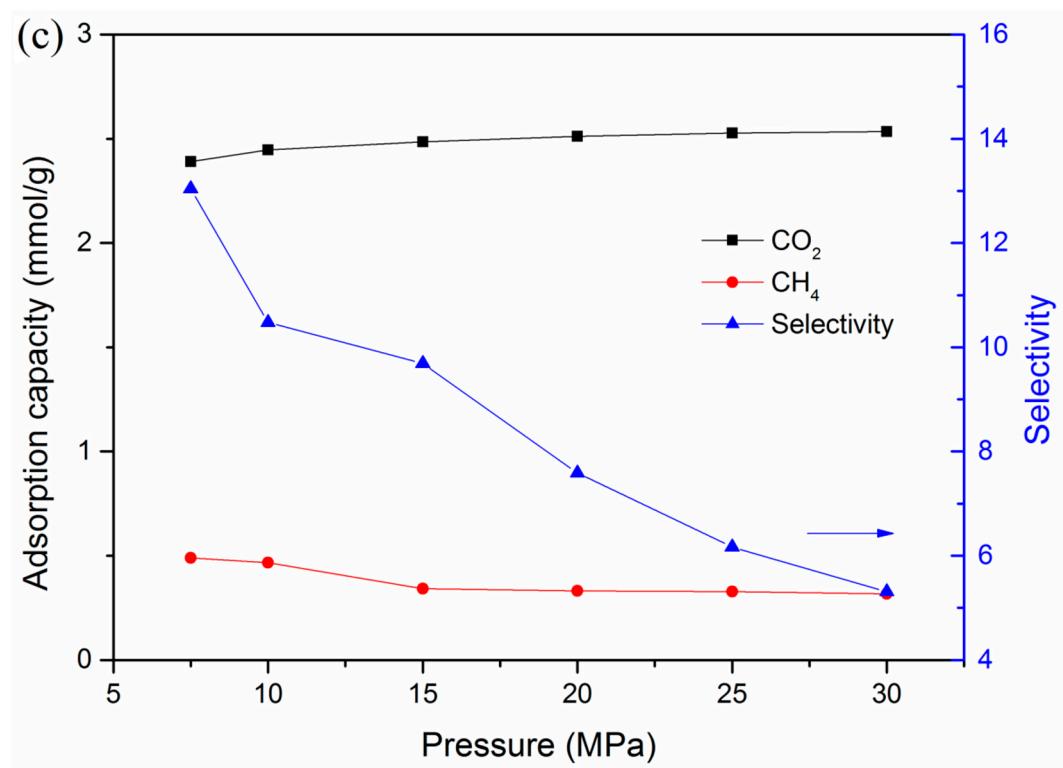
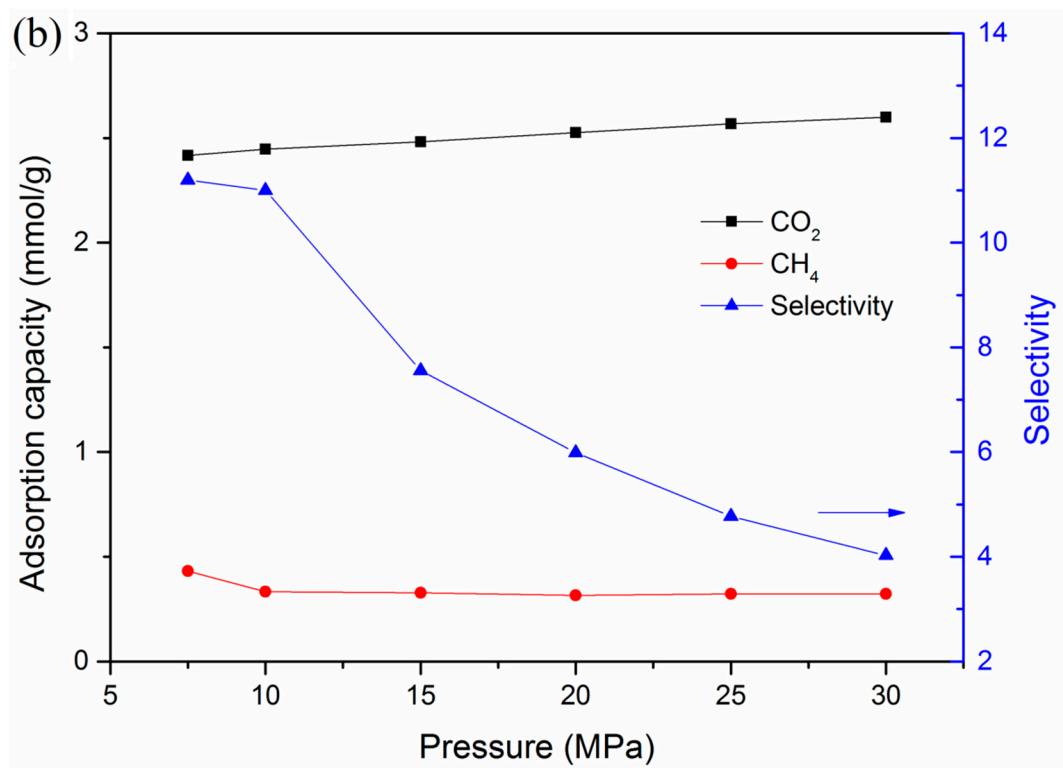


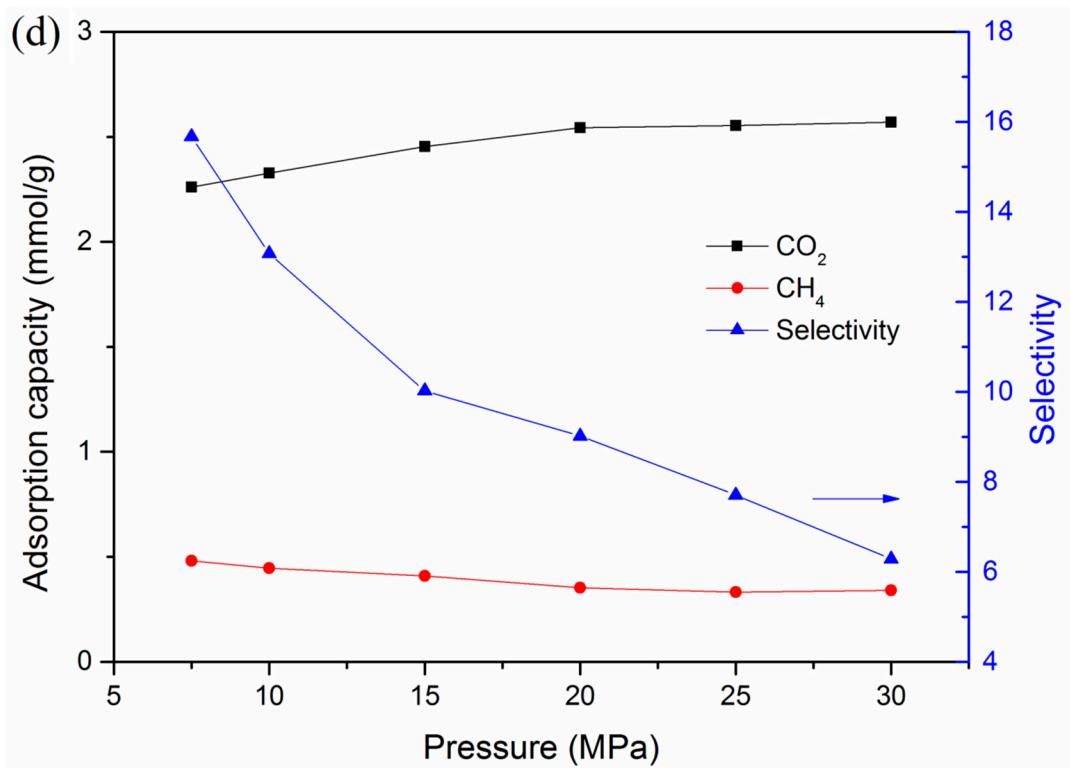




**Figure S1.** The adsorption isotherms of pure  $\text{CH}_4$  at different temperatures and Langmuir fitting in kerogen with different maturity levels: (a) I-A; (b) II-B; (c) II-C; (d) II-D.







**Figure S2.** Variation of adsorption capacities and selectivity of  $\text{CO}_2/\text{CH}_4$  binary mixture as a function of  $\text{CO}_2$  partial pressure at different  $\text{CH}_4$  fixed partial pressures: (a) 5 MPa; (b) 15 MPa; (c) 20 MPa; (d) 25 MPa,  $T=298\text{ K}$ .