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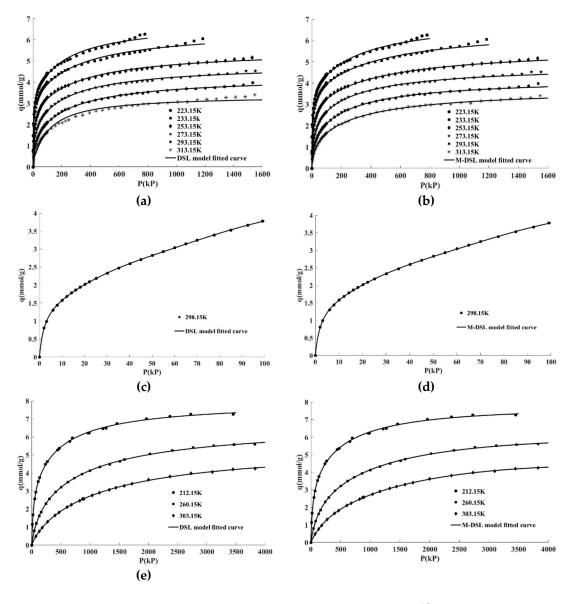
Modified Dual-Site Langmuir Adsorption Equilibrium Models from A GCMC Molecular Simulation

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Received: 16 January 2020; Accepted: 11 February 2020; Published: 14 February 2020



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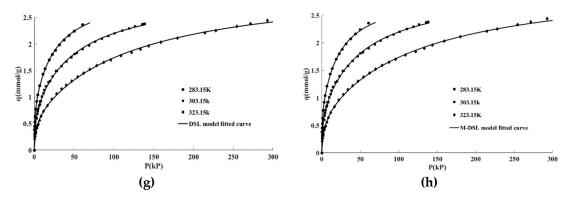


Figure S1. Comparison curves of the DSL model and the M-DSL model for different systems, (**a**) The DSL model for C2H4-HHPAC; (**b**) the M-DSL model for C2H4-HHPAC; (**c**) the DSL model for CO2-MIL-101(Cr); (**d**) the M-DSL model for CO2-MIL-101(Cr); (**e**) the DSL model for CH4-BPL; (**f**) the M-DSL model for CH4-BPL; (**g**) the DSL model for CO2-H-Mordenite; (**h**) the M-DSL model for CO2-H-Mordenite.

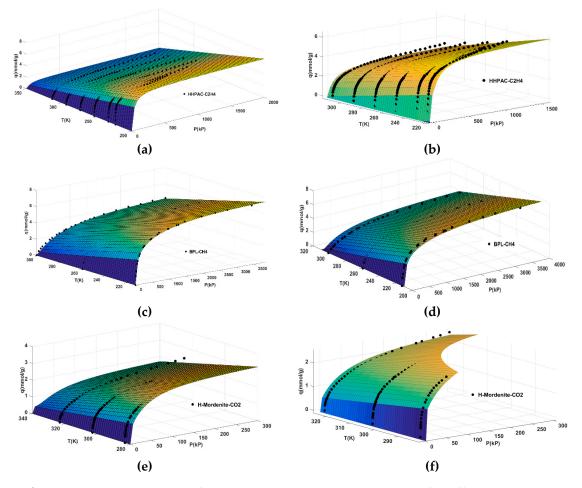


Figure S2. Comparison curves of the TDSL model and the M-TDSL model for different systems, (a) The TDSL model for C₂H₄-HHPAC; (b) the M-TDSL model for C₂H₄-HHPAC; (c) the TDSL model for CH₄-BPL; (d) the M-TDSL model for CH₄-BPL; (e) the TDSL model for CO₂-H-Mordenite; (f) the M-TDSL model for CO₂-H-Mordenite.