

单壁碳纳米管上毒性苯气体净化的分子模拟

彭 璇*

(北京化工大学信息科学与技术学院, 北京 100029)

Molecular Simulations of the Purification of Toxic Benzene Gas on Single-Walled Carbon Nanotubes

PENG Xuan*

(College of Information Science and Technology, Beijing University of Chemical Technology, Beijing 100029, P. R. China)

*Corresponding author. Email: pengxuan@mail.buct.edu.cn, pengxuan@126.com; Tel: +86-10-64430917.

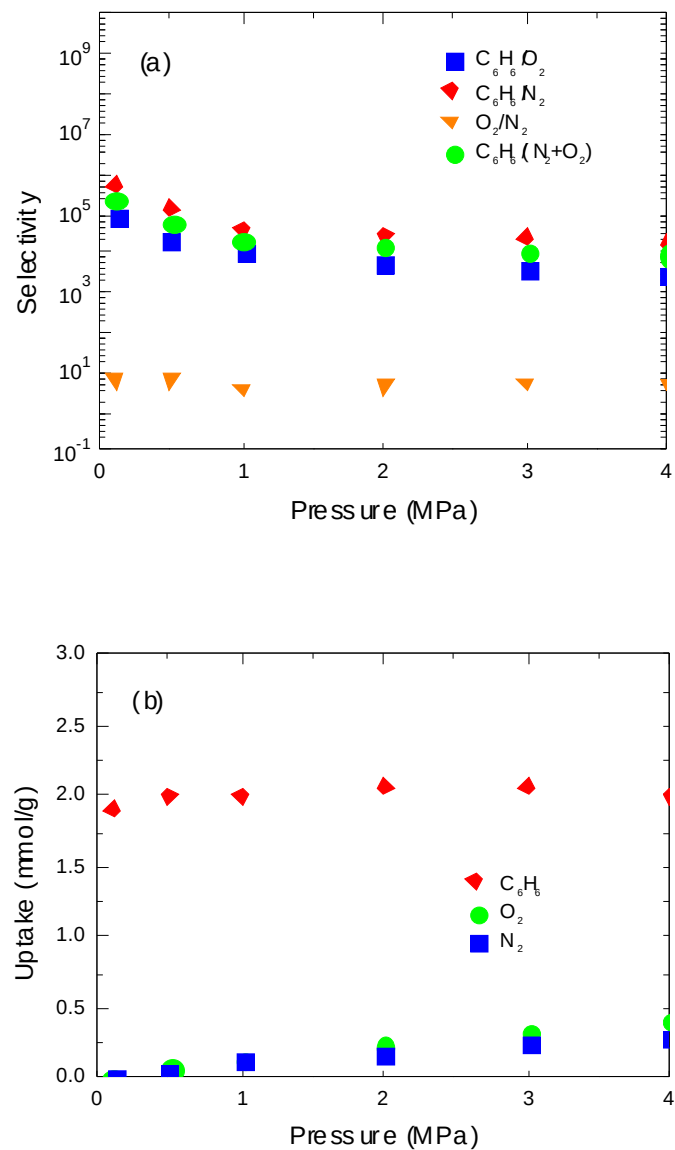


Fig.S1 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures

($y_{\text{N}_2}=0.79$ and $y_{\text{C}_6\text{H}_6}=0.0003$) in (08,08) SWNTs at 303 K

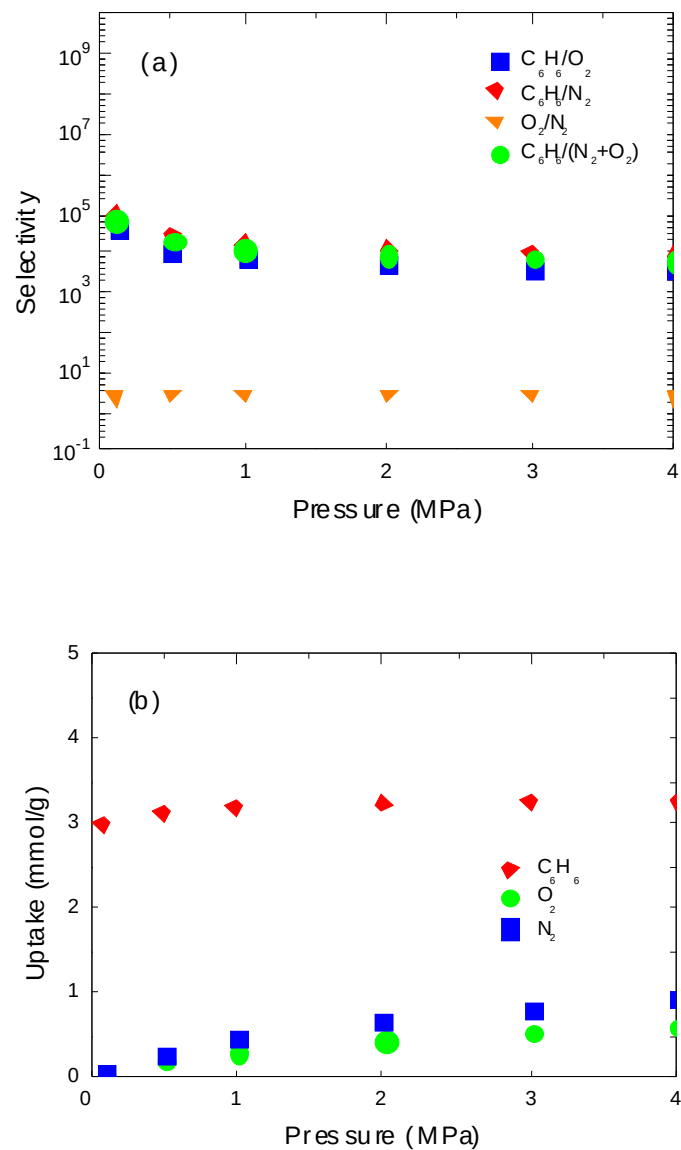


Fig.S2 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures

($y_{\text{N}_2}=0.79$ and $y_{\text{C}_6\text{H}_6}=0.0003$) in (10,10) SWNTs at 303 K

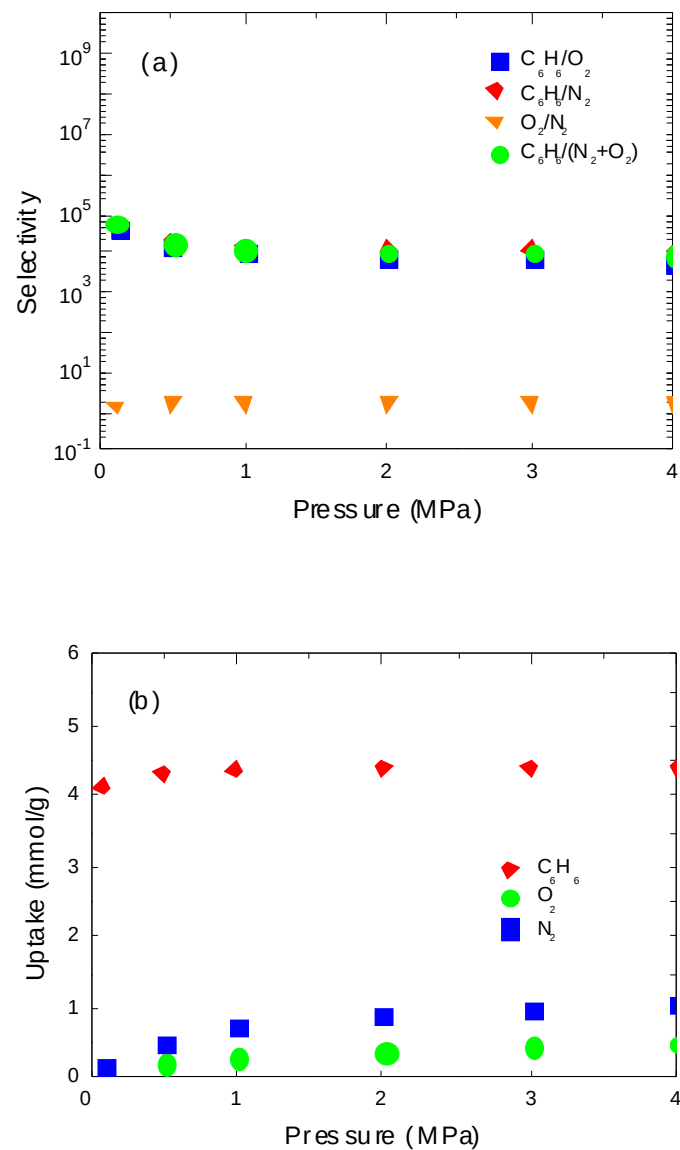


Fig.S3 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures

($y_{\text{N}_2}=0.79$ and $y_{\text{C}_6\text{H}_6}=0.0003$) in (12,12) SWNTs at 303 K

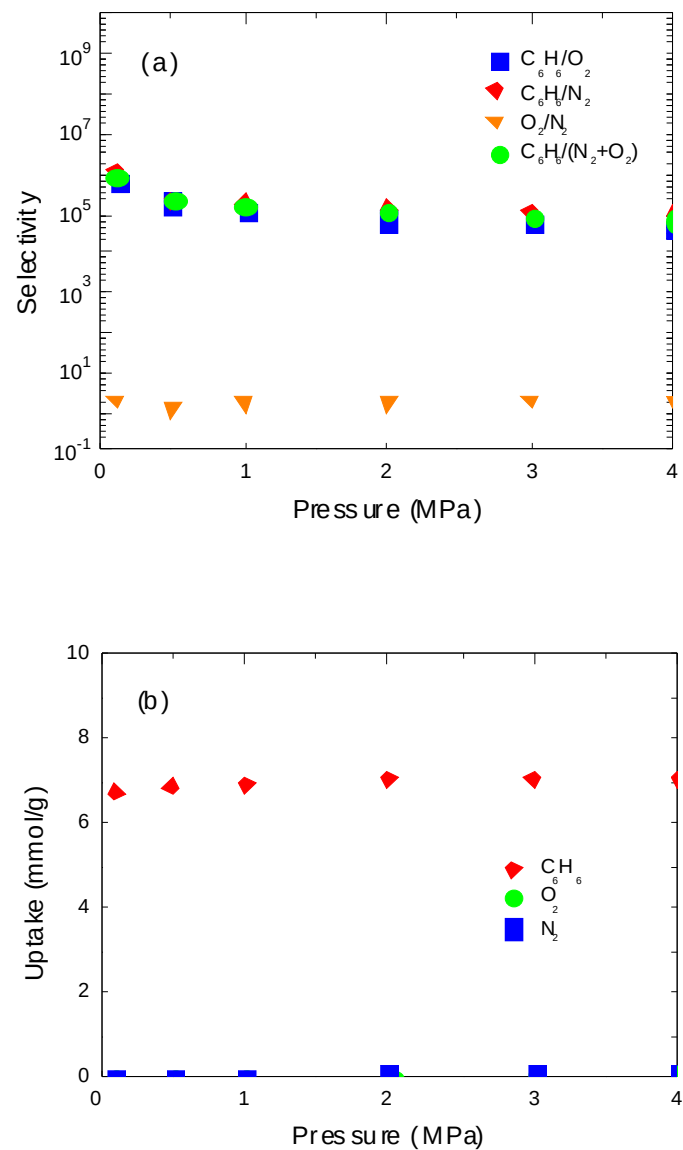


Fig.S4 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures ($y_{\text{N}_2}=0.79$ and $y_{\text{C}_6\text{H}_6}=0.0003$) in (15,15) SWNTs at 303 K

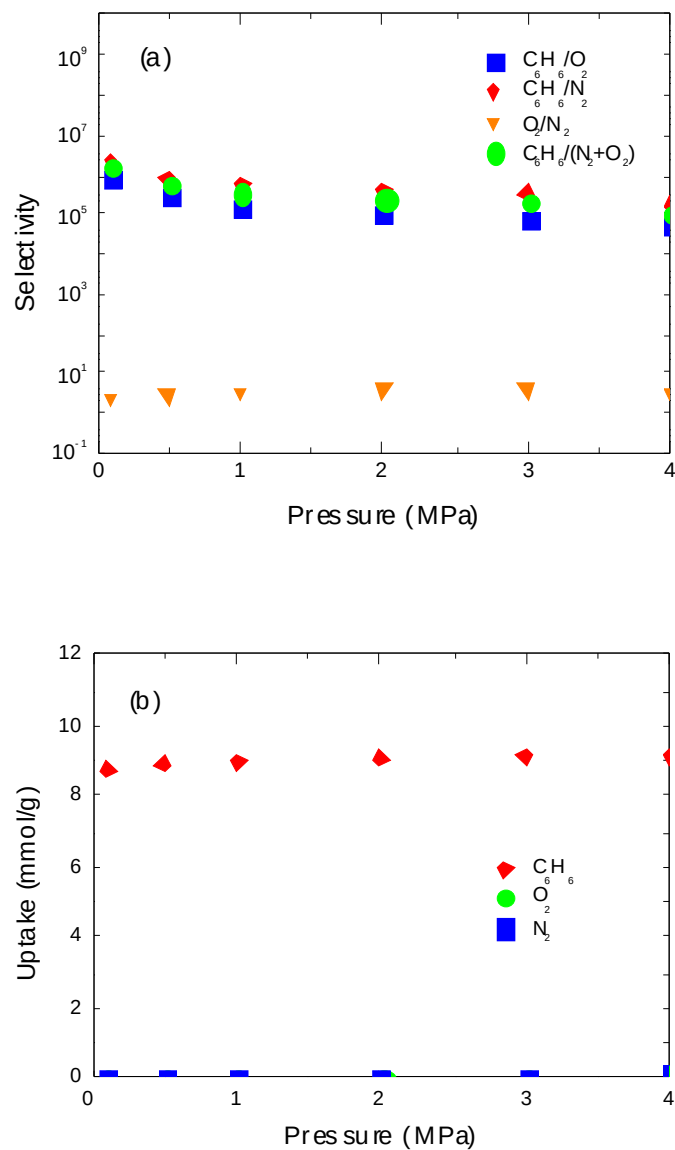


Fig.S5 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures ($y_{N_2}=0.79$ and $y_{C_6H_6}=0.0003$) in (18,18) SWNTs at 303 K

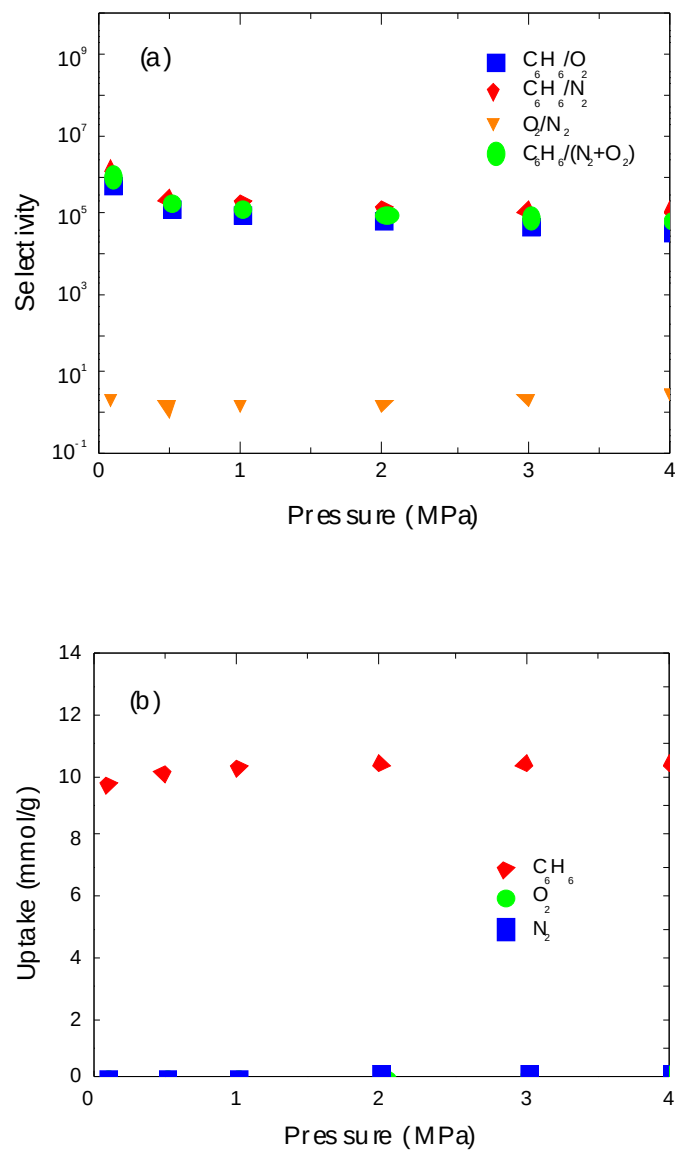


Fig.S6 Adsorption selectivities and isotherms of N_2 - O_2 - C_6H_6 ternary mixtures ($y_{N_2}=0.79$ and $y_{C_6H_6}=0.0003$) in (20,20) SWNTs at 303 K