

POSS-Based Luminescent Porous Polymers for Carbon Dioxide Sorption and Nitroaromatic Explosives Detection

*Dengxu Wang,^{a,b} Liguo Li,^b Wenyang Yang,^b Yujing Zuo,^b Shengyu Feng,^{*a,b} and*

*Hongzhi Liu^{*b}*

^a National Engineering Technology Research Center for Colloidal Materials,
Shandong University, Jinan 250100, P. R. China

^b Key Laboratory of Special Functional Aggregated Materials & Key Laboratory of
Colloid and Interface Chemistry (Shandong University), Ministry of Education,
School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100,
P. R. China

*Corresponding Authors. Tel: +86 531 88364866; Fax: +86 531 88564464. E-mail:
fsy@sdu.edu.cn; liuhongzhi@sdu.edu.cn.

Table of contents:

Fig. S1 Energy dispersive spectroscopy of LHPP-1~LHPP-3

Fig. S2 FTIR spectra enlarged from 1800 cm^{-1} to 1200 cm^{-1} of OVS and LHPP-1

Fig. S3 BET plots of LHPP-1 (top, $r = 0.999968$, $C = 375.87$), LHPP-2 (middle, $r = 0.999966$, $C = 857.19$) and LHPP-3 (bottom, $r = 0.999992$, $C = 190.22$)

Fig. S4 XRD patterns of LHPP-1 to LHPP-3

Fig. S5 FE-SEM images of LHPP-2 (left) and LHPP-3 (right).

Fig. S6 Fluorescent spectra of triphenylamine in the solid state and in THF solution excited at 310 nm

Fig. S7 HOMO and LUMO orbital diagrams of LHPPs. The molecular orbital calculations were performed with the Gaussian 03 program at the B3LYP/6-31G (d) level.¹

Fig. S8 Stern-Volmer plots of LHPP-3. (a) NT, $R=0.9934$; (b) DNT, $R=0.9833$; (c) TNT, $R=0.9636$

Fig. S9 HOMO and LUMO calculations for LHPP-3, NT, DNT and TNT. The molecular orbital calculations were performed with the Gaussian 03 program at the B3LYP/6-31G (d) level.¹

Table S1 HOMO and LUMO energies of LHPP-3, NT, DNT and TNT

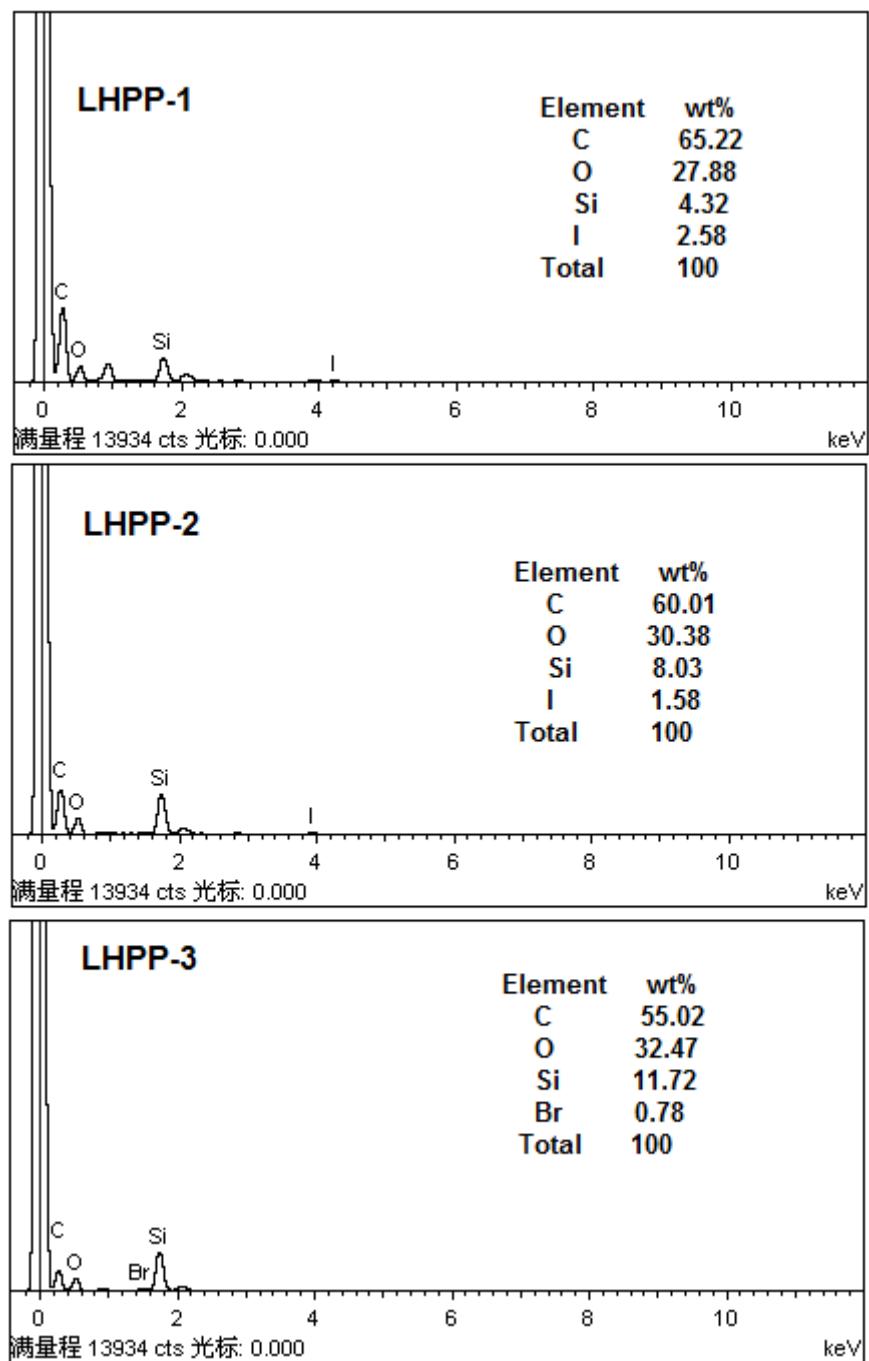


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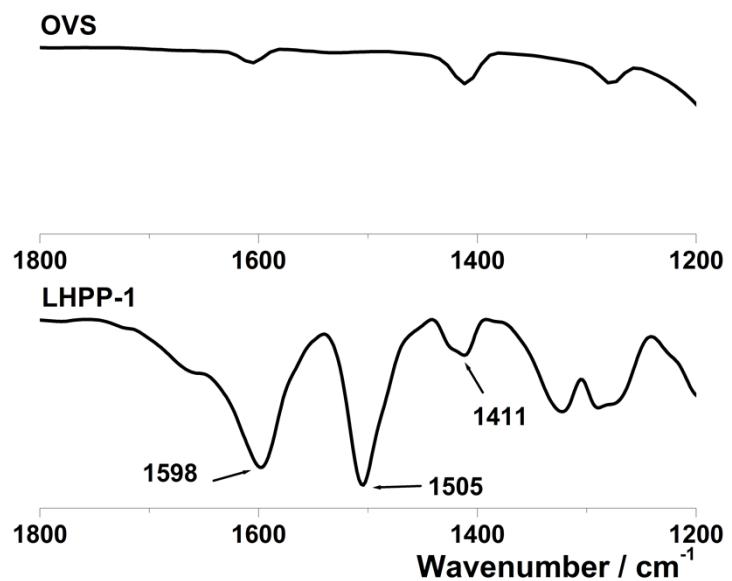


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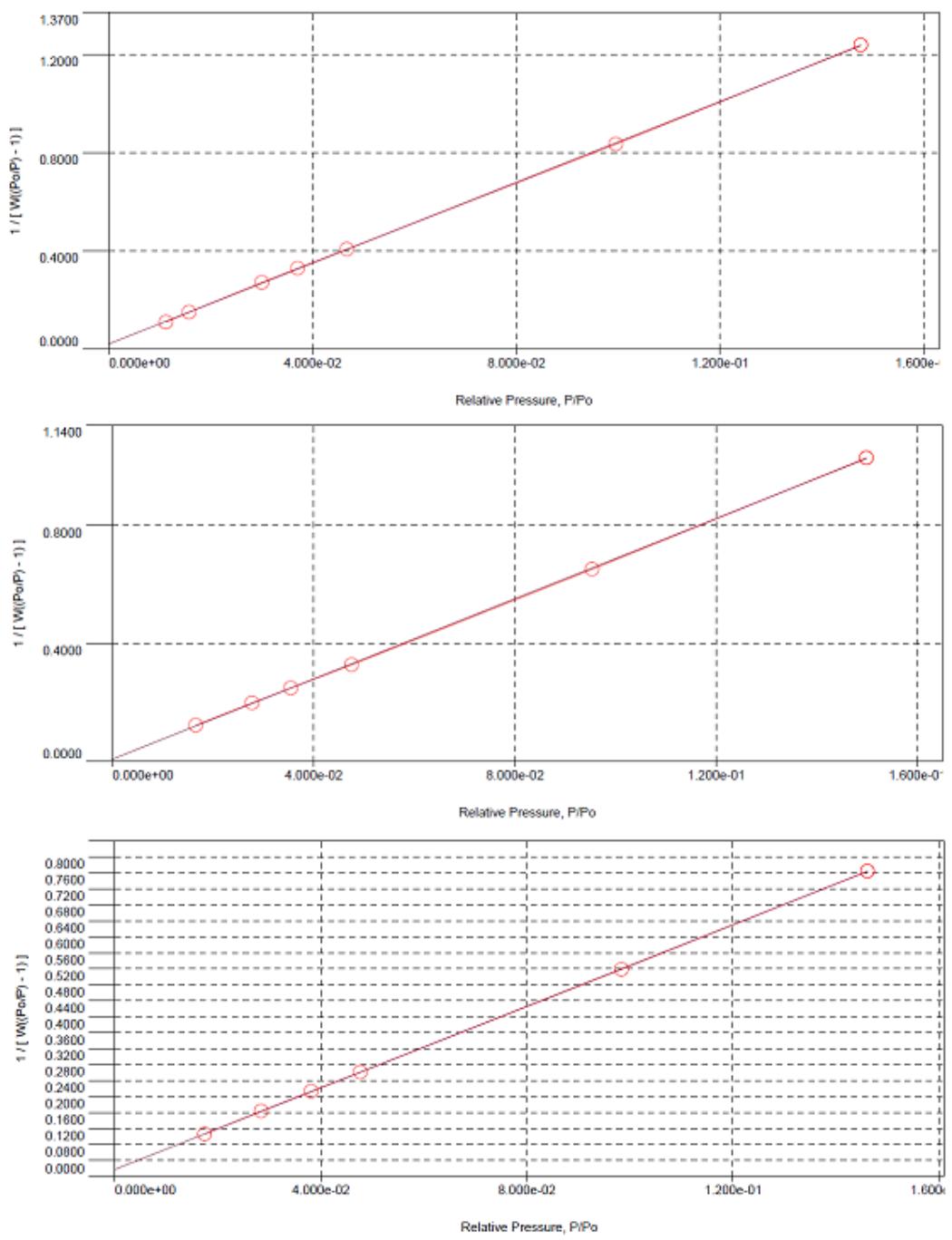


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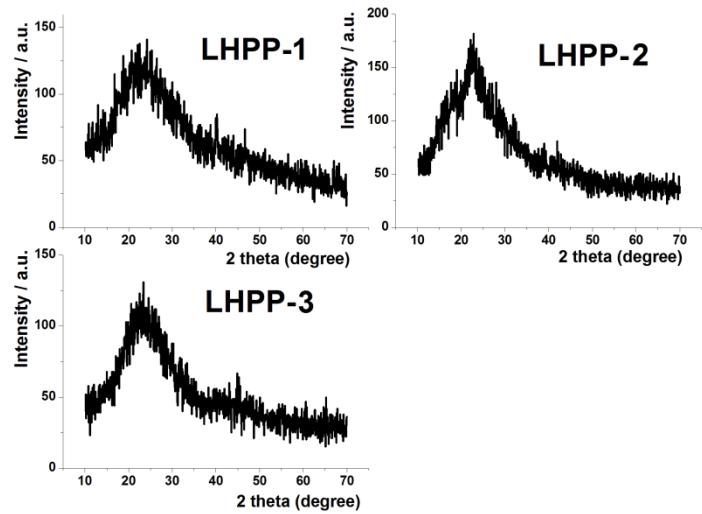


Fig. S4 XRD patterns of LHPP-1 to LHPP-3

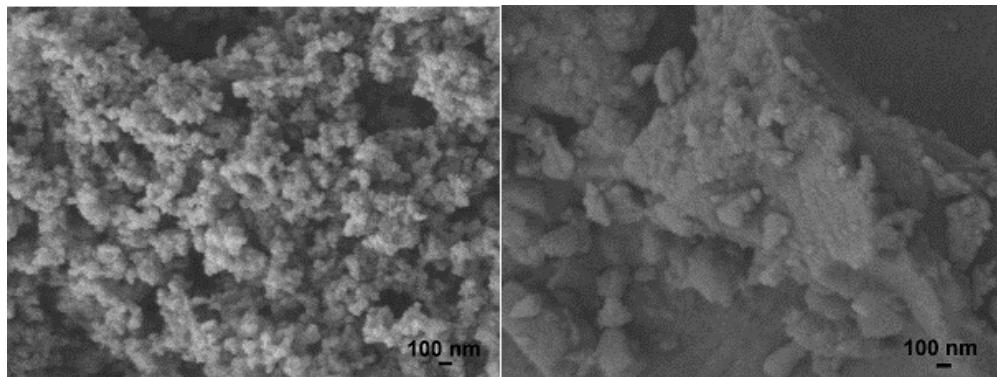


Fig. S5 FE-SEM images of LHPP-2 (left) and LHPP-3 (right).

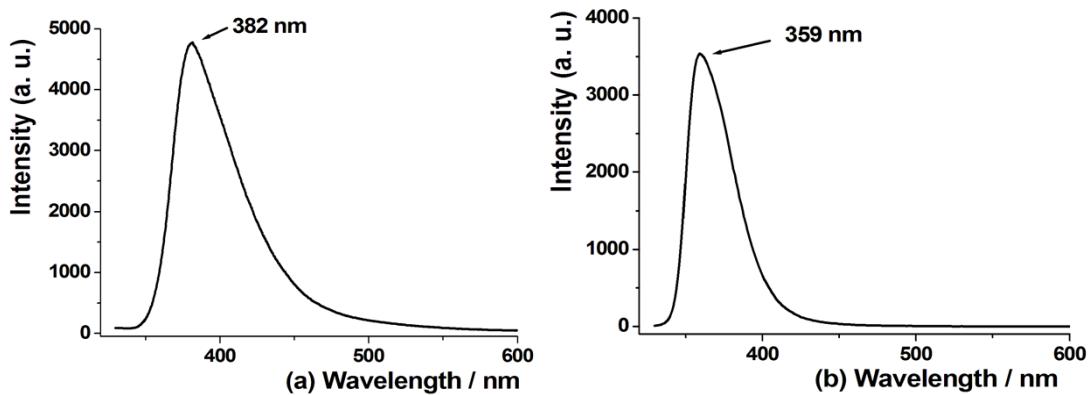


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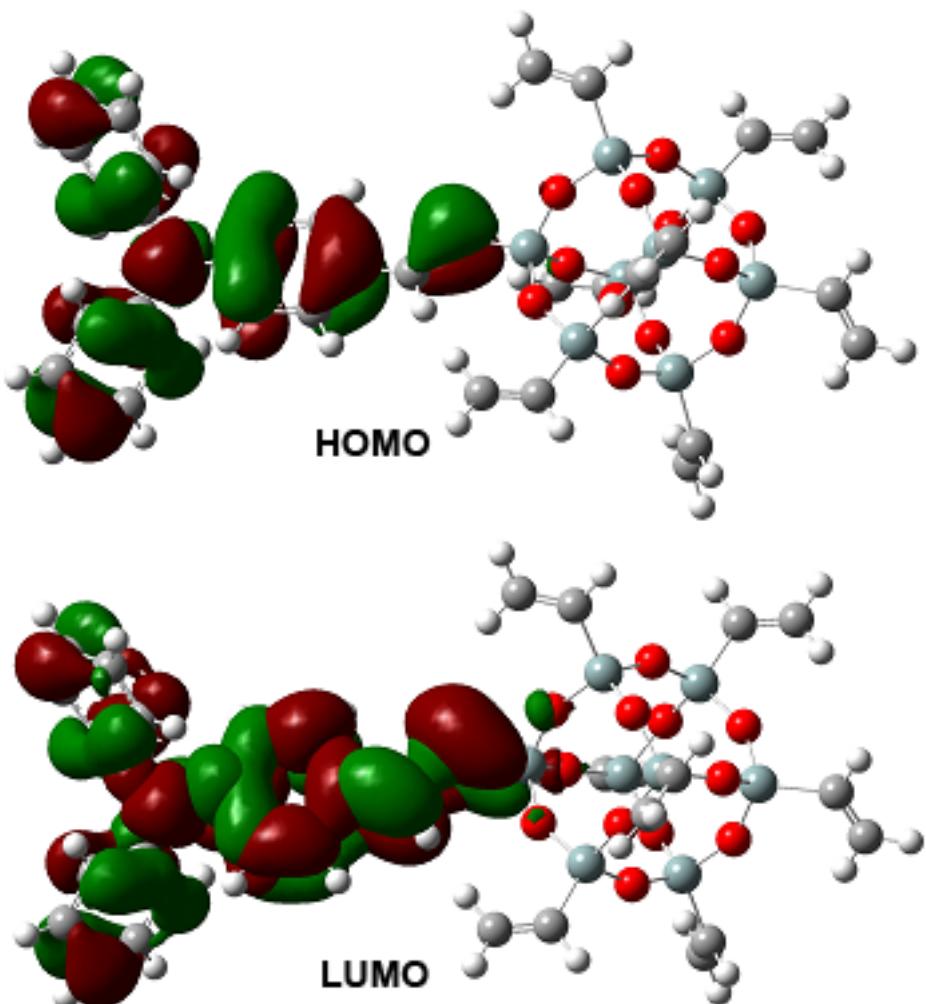


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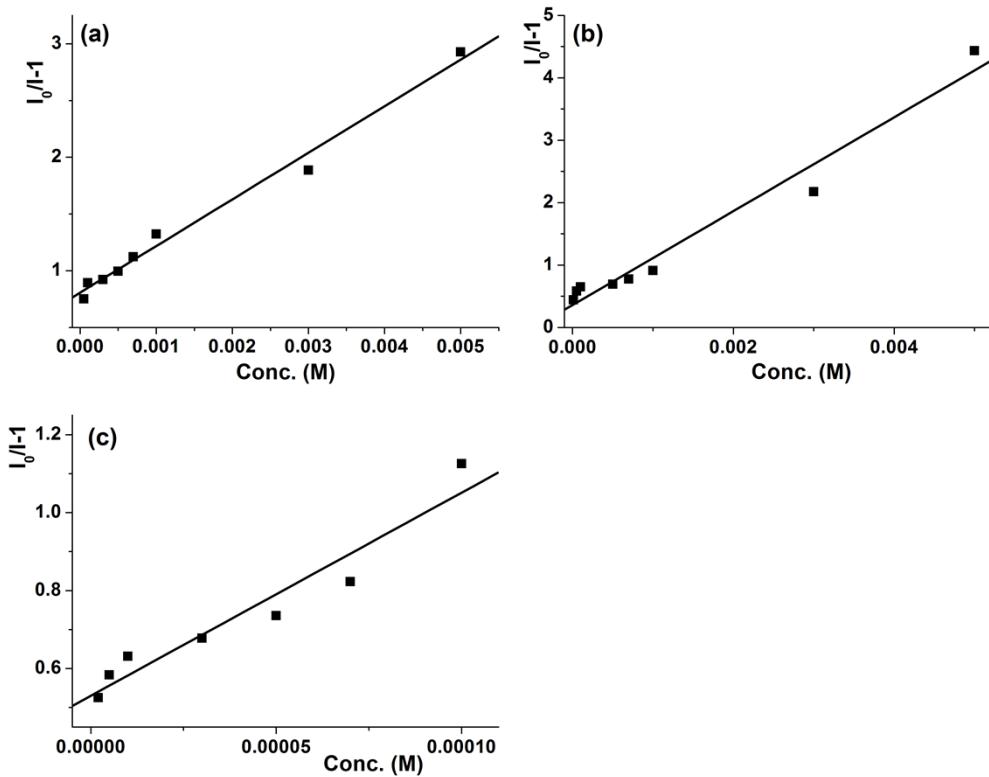


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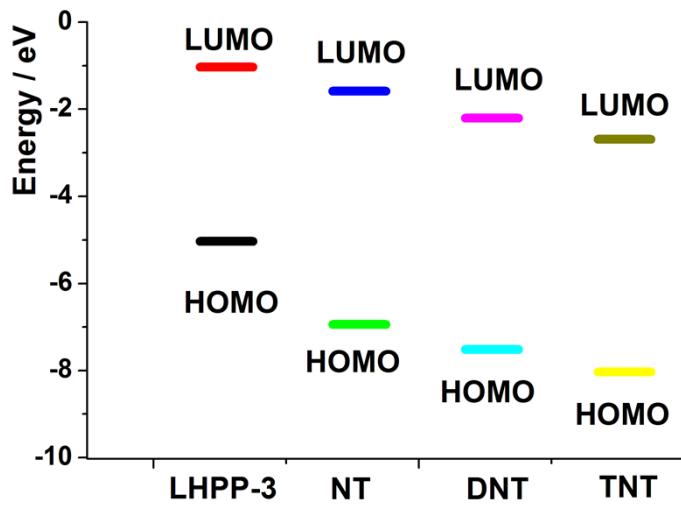


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Table S1. HOMO and LUMO energies of LHPP-3, NT, DNT and TNT

MO energy / eV	LHPP-3	NT	DNT	TNT
HOMO	-5.55	-6.94	-7.51	-8.03
LUMO	-1.01	-1.58	-2.20	-2.69

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Revision B.04 2003 (Gaussian, Inc.: Pittsburgh, PA).