

Mechanistic Implications of Au_n/Ti-Lattice Proximity for Propylene Epoxidation

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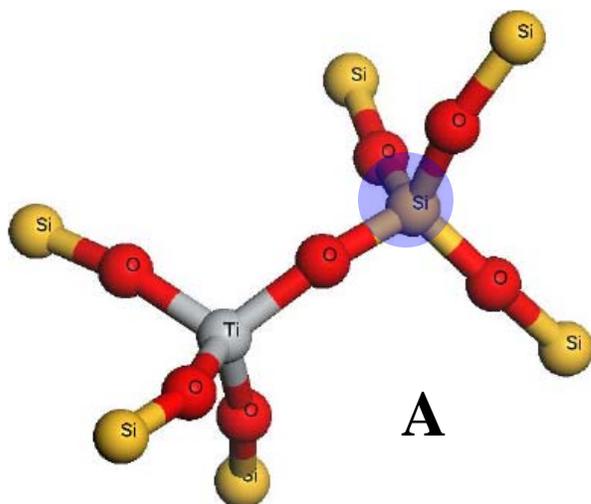
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Supporting Information:

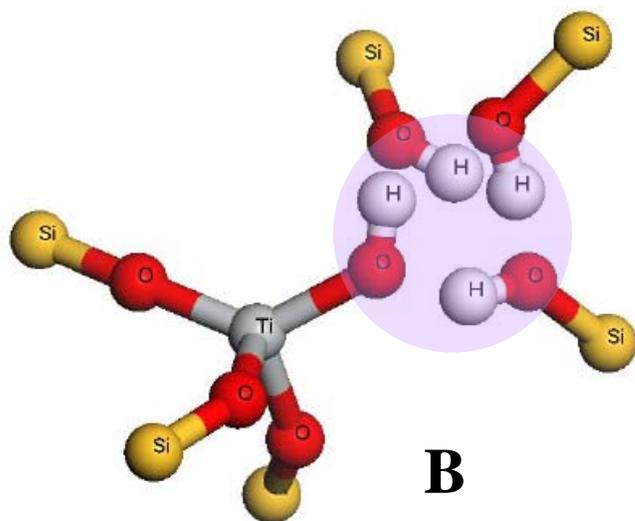
A complete citation for the reference 38 is included here:

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

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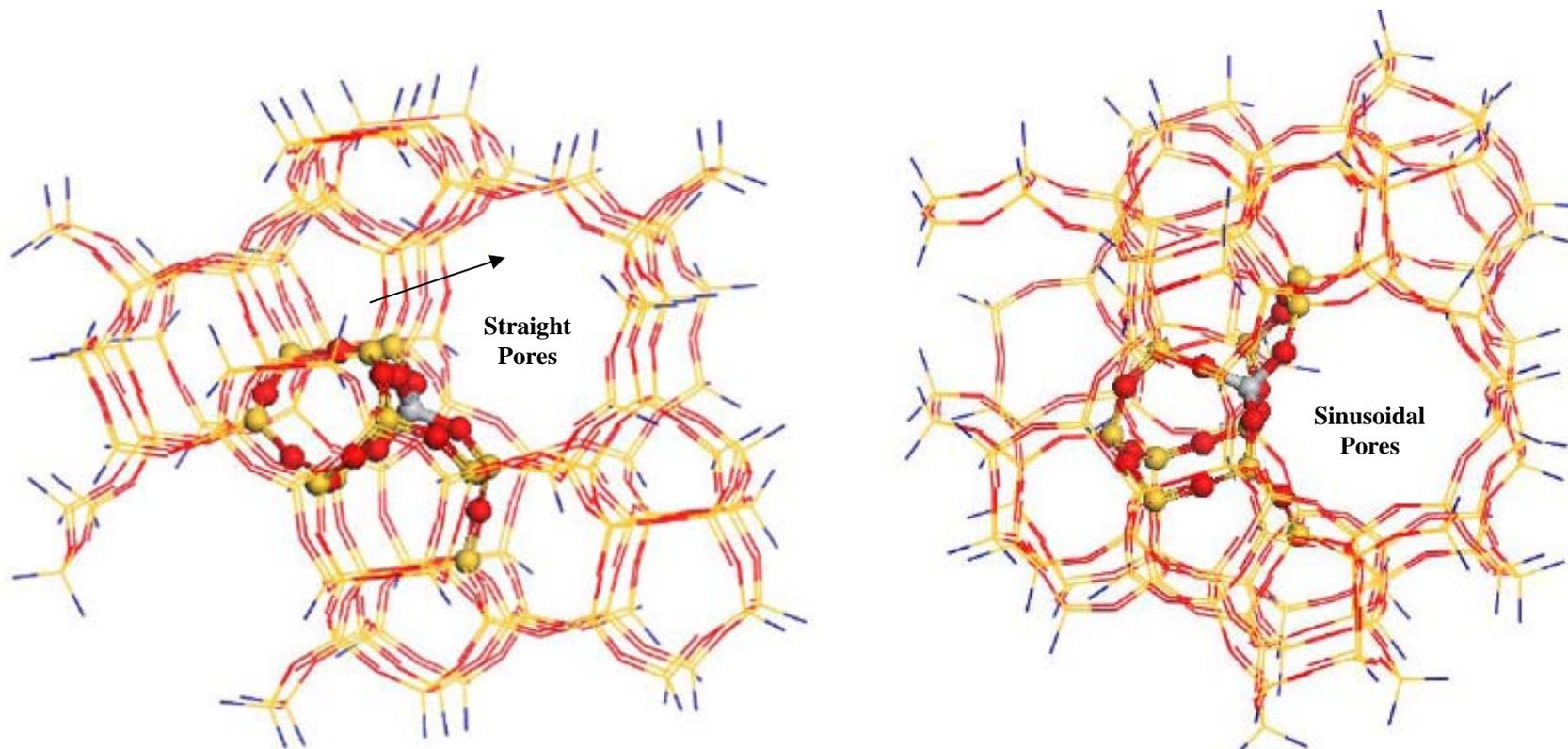


A



B

A schematic view of a fully tetrahedrally bonded Ti ion substituted for a Si ion at one of the lattice positions of TS-1 (A) and the same Ti site located near a silicon vacancy terminated with hydroxyl groups forming a silanol nest (B).



An embedded-cluster model (119 T sites) of the TS-1 lattice. The QM region is made up of 11 T sites and is represented by the ball and stick display format. The MM region is made up of 108 T sites and is represented by the wire-mesh format. The MM region has terminal H atoms at the periphery.

Ti atom: Grey Ball, Si atoms: Yellow Balls and Wires, O atoms: Red Balls and Wires, H atoms: Blue Wires