



















- [31] M. Digne, P. Sautet, P. Raybaud, P. Euzen, H. Toulhoat, *J. Catal.* 226 (2004) 54-68.
- [32] M.C. Valero, P. Raybaud, P. Sautet, *J. Phys. Chem. B* 110 (2006) 1759-1767.
- [33] M. Digne, P. Raybaud, P. Sautet, B. Rebours, H. Toulhoat, *J. Phys. Chem. B* 110 (2006) 20719-20720.
- [34] T. Taniike, M. Tada, Y. Morikawa, T. Sasaki, Y. Iwasawa, *J. Phys. Chem. B* 110 (2006) 4929-4936.
- [35] H.P. Pinto, R.M. Nieminen, S.D. Elliott, *Phys. Rev. B* 70 (2004) 125402.
- [36] A. Dyan, P. Cenedese, P. Dubot, *J. Phys. Chem. B* 110 (2006) 10041-10050.
- [37] J. Handzlik, P. Sautet, *J. Catal.* 256 (2008) 1-14.
- [38] C. Wolverton, K.C. Hass, *Phys. Rev. B* 63 (2000) 024102.
- [39] G. Paglia, C.E. Buckley, A.L. Rohl, B.A. Hunter, R.D. Hart, J.V. Hanna, L.T. Byrne, *Phys. Rev. B* 68 (2003) 144110.
- [40] G. Paglia, A.L. Rohl, C.E. Buckley, G.D. Gale, *Phys. Rev. B* 71 (2005) 224115.
- [41] L. Smrcok, V. Langer, J. Krestan, *Acta Cryst. C* 62 (2006) i83-i84.
- [42] P. Souza Santos, H. Souza Santos, S.P. Toledo, *Mater. Res. Ibero-Am. J.* 3 (2000) 104-112.
- [43] P. Manivasakan, V. Rajendran, P.R. Rauta, B.B. Sahu, B.K. Panda, *Powder Technol.* 211 (2011) 77-84.
- [44] M.L. Guzmán-Castillo, E. López-Salinas, J.J. Fripiat, J. Sánchez-Valente, F. Hernández-Beltrán, A. Rodríguez-Hernández, J. Navarrete-Bolaños, *J. Catal.* 220 (2003) 317-325.
- [45] H. Sun, *J. Phys. Chem. B* 102 (1998) 7338-7364.
- [46] S. Grimme, *J. Comput. Chem.* 27 (2006) 1787-1799.
- [47] B. Delley, *J. Chem. Phys.* 92 (1990) 508-517.
- [48] B. Delley, *J. Chem. Phys.* 113 (2000) 7756-7764.