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DFT study of the Ni particle size on CH_4/CO_2 reforming over Ni/MgO catalyst

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Carbon deposition, as the main cause of supported Ni catalysts in CH_4/CO_2 reforming, is sensitive to the metal Ni particle size. To explore what's the reason of the particle size effect during the catalysis process, Ni clusters, Ni4, Ni8 and Ni12 which reflect the different cluster thicknesses supported on the MgO (100) slabs, have been adapted to simulate Ni/MgO catalysts. By using density functional theory (DFT), the reaction pathways of CH_4/CO_2 reforming on Nix/MgO (100) models are used to investigate the particle size that might affect the reaction pathway. The reforming mechanisms of CH_4/CO_2 on different Nix/MgO (100) indicate the energy barriers of CH_4 dissociated adsorption, CH dissociation and C oxidation three factors are all declining with the decrease of the Ni cluster size. The Hirshfeld charges analyses of those three steps show only atoms of Nix cluster on bottom or second bottom layer can obtain electrons from the MgO supporter and the main electrons transferring are occurring between adsorbed species and the Ni atoms in surface layer. The Ni atoms of surface layer in small Ni cluster will have more electrons and have better catalytic activity. As a result, the NiO/MgO catalysts with small Ni particle would expose more Ni atoms in contact with the MgO supporter, which might be the reason of metal particle size effect.

Biography

Wen-ying Li is a Coal Chemical Engineering from Taiyuan University of Technology, China and Distinguished Professor Cheung Kong Scholars Program. Her research field Coal Chemistry, Coal pyrolysis, Coal-based energy integration system. She completed her Ph.D. in 1995, Organic Chem. Eng., Dalian University of Technology, China, M.E. in 1992, Organic Chem. Eng., Taiyuan University of Technology, China and she completed her B.E. in 1989, Coal Chem. Eng., Taiyuan University of Technology, China. She has published more than 20 papers in reputed journals.

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