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Surface analysis of the *ab*-plane of $MoVTeNbO_x$ catalysts for propane (amm)oxidation by Low Energy Ion Scattering (LEIS)

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At present, there is great global interest in utilization of light alkane feedstocks in the production of petrochemicals by selective (amm)oxidation due to current abundance and lower costs of alkanes compared to the corresponding olefins. However, direct oxidation of alkanes requires multifunctional catalysts that cope with simultaneous activation of C-H bonds, molecular oxygen and ammonia and that concurrently provide selectively oxidizing oxygen atoms. For selective oxidation of propane to acrylic acid and ammoxidation to acrylonitrile, this multi-functionality is implemented in chemically and structurally complex $MoVTeNbO_x$ catalysts, which show high activities and selectivities to acrylic acid and acrylonitrile. Usually, these catalysts consist of phase mixtures composed of the so-called "M1" and "M2" phases, as well as minor phases, like Mo_5O_{14} type structures and binary MoV and MoTe compounds. Propane activation and high selectivities to acrylic acid and acrylonitrile are generally attributed to the presence of the orthorhombic M1 phase. However, the essential presence of all four elements for catalytic activity is a matter of ongoing discussions. It has been suggested [1] that the *ab*-planes of the M1 phase contain the active and selective surface sites.

In this study we address the role of the *ab* planes of the M1 phase in propane (amm)oxidation by investigating the topmost surface composition and catalytic behavior of a pure M1 phase preferentially exposing this catalytic surface. Phase-pure M1 catalysts exhibiting rod-like crystal morphology in which the bulk *ab* planes were oriented normal to the long rod axis were prepared hydrothermally. The following three M1 catalysts were investigated: (i) the original M1 catalyst after a thermal treatment in nitrogen at 600^{o}C; (ii) the original catalyst after its external surface was passivated by silylation; and (iii) the passivated catalyst after a thorough comminution to selectively expose the *ab* planes. The catalytic role of the *ab* planes of the M1 phase was investigated by combining the microreactor study of propane (amm)oxidation over these model M1 catalysts with Low Energy Ion Scattering (LEIS) to selectively determine the atomic composition of outer surface of the *ab*-planes.

[1] V.V. Guliants, R. Bhandari, R.S. Soman, O. Guerrero-Perez, M.A. Banares, Appl. Catal. A 274 (2004) 213.