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Catalytic activity of supported $LaMnO_3$ for methane oxidation

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$LaMnO_3$ reveals very high catalytic activity for methane combustion. Samples with the highest specific activity had the surface area 20-30 m^2/g and were obtained by nano-technology methods (sol-gel processes, flame pyrolysis and flame hydrolysis). The alternative technique for synthesis of nano-size oxides consists in dispersion of active material on support with high surface area. This procedure is easier and more efficient in comparison with methods of nano-technology. In the present work, we compared catalytic characteristics of $LaMnO_3$ (5-20 mol%) supported on lanthana, Mn_2O_3, MgO and the same parameters of individual substrates. Mn-perovskite formed on support as a result of chemical interaction between carrier and metal oxide(s).The last one(s) formed at heat treatment of powder support impregnated by La and Mn nitrate solutions.

The rate constant for sample $LaMnO_3$/MgO with 5% at 550°C achieved 845 μmol/bar·s·g_{LaMnO3} (845 rc-unites) and exceeded the same characteristic for individual $LaMnO_3$ (20 m^2/g), having the highest catalytic activity (700 rc-unites). It was revealed that increase of concentration leaded to decreasing of the rate constant down to 476 rc-unites as a result of agglomeration of nano-size particles supported $LaMnO_3$. Samples $LaMnO_3/Mn_2O_3$ showed similar behaviour but the values of the rate constant in this case were lower. This fact correlated with support surface area. The experimental data concerned to lanthana in contrast to MgO and Mn_2O_3 showed that activities of supported catalysts and pure support were comparable and there were some difficulties to calculate activity referred to $LaMnO_3$.

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Field-induced electron density redistribution at carbon surface: many body effects

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Increasing interest to the field emission applications of the carbon nanotubes and other nanosized carbon formations stimulates the theoretical studies of the electron density distributions near the carbon surfaces. In present contribution a new approach is proposed for the calculations of the field-free and field-modified electron density distributions at a semi-infinite carbon crystal using the functional integration method [1]. This approach allows correct considering of the exchange-correlation effects and makes possible the proper field-effect account for broad field ranges without to use the perturbation theory. The electron-ion interaction is described by a nonlocal model pseudopotential of Kleinman-Bylander type.

The results of calculations are compared to the field-ion microscopic measurements of local electrostatic fields in the immediate vicinity of individual surface atoms. The implications of the obtained results on the particular fields of nanotechnology and heterogeneous catalysis, are discussed.

[1] P.P.Kostrobiy, B.M.Markovych, Condensed Matter Physics, 6 (2003) 347

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Catalytic activity for methane flameless combustion and thermal stability of nano-sized lanthanum cobaltites doped with Ce, Pr and Tb

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High surface area nano-sized catalysts with general formula $La_{0.9}M_{0.1}CoO_3$ (M=Ce, Pr, Tb) were synthesised by a novel flame-spray-pyrolysis method, based on spraying a solution of the corresponding metals salts (acetates in the present case, dissolved in propionic acid), together with oxygen, in a nozzle burner, where the mixed oxides particles form, followed by collection of the latter by means of an electrostatic precipitator.

All the prepared samples possessed the $LaCoO_3$ perovskite-like structure and consisted of 30-60 nm particles, lumped into larger (80-200 nm) agglomerates. Their surface area ranged from 45 to 60 m^2/g. All of the catalysts showed a very high activity for the methane flameless combustion, attaining 100% conversion at a temperature T_f (temperature of full conversion) ranging between 495 and 515°C, depending on the nature of the M doping ions. The results of life-tests did not show any decreasing of catalytic activity after 50 h under reaction conditions at T_f. Thermal stability under high temperature exploitation was investigated by overheating the catalysts two times for 1h at 800°C in flowing reacting gas mixture (fast deactivation cycles) and then measuring again methane conversion at T_f. All the catalysts showed a more or less considerable decrease of activity, depending on chemical composition. For example, conversion after the second cycle decreased from 100% down to 80% for $LaCoO_3$ and to 48% for $La_{0.9}Tb_{0.1}CoO_3$. Taking into account the results of SEM analysis, this was attributed to sintering, connected with Gibbs instability of nano-sized materials.