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Negative-Ion Catalysis of Methane to Methanol without CO_2 Emission[1] A. TESFAMICHAEL, K. SUGGS, Z. FELFLI, A.Z. MSEZANE, Clark Atlanta University — We have carried out a theoretical investigation of the catalytic activities of the atomic Y^-, Ru^-, At^-, In^-, Pd^-, Ag^-, Os^- and Pt^- ions for the selective partial oxidation of methane to methanol without CO_2 emission. The objective was to identify effective atomic negative ion catalysts using the data for the atomic Au^- ion as the benchmark. The role of the atomic negative ions in catalysis is essentially to disrupt the C-H bonding in CH_4 oxidation thereby eliminate the competition from the carbon dioxide formation [1]. Dispersion-corrected density-functional theory has been used for the investigation. From the energy barrier calculations and the thermodynamics of the reactions, we conclude that the catalytic effect of the atomic Ag^-, At^-, Ru^-, and Os^- ions is higher than that of the atomic Au^- ion catalysis of CH_4 conversion to methanol. By controlling the temperature around 290, 300, 310, 320 and 325 K methane can be completely oxidized to methanol without the emission of the CO_2 through the atomic Os^-, Ag^-, At^-, Ru^- and Au^- ion catalysts, respectively. We conclude by recommending the investigation of the catalytic activities of combinations of the above negative ions for significant enhancement of the selective partial oxidation of methane to methanol.

[1] A. Z. Msezane *et al, Gold Bull.* **45**, 17 (2012)

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