Theoretical insight into methane oxidation to methanol on Fe-embedded functionalized graphene as a promising catalyst
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Abstract: Methane oxidation on Fe single atom embedded on pyridinic-N supported on graphene (Fe@N4G) has been investigated by density functional theory (DFT) calculations. Reaction pathways through both Eley-Rideal (ER) and Langmuir-Hinshelwood (LH) mechanisms of methane oxidation are explored in detail. The reaction starts with N₂O chemically adsorbing on Fe-N4G to produce N₂ gas and oxo–Fe@N4G (O–Fe@N4G). The charge transfer from surface to O atom at O–Fe@N4G makes this O atom very reactive to oxidize methanol, confirmed by the Bader charge analysis. One of the C-H bonds of methane dissociative to produces CH₃ and OH strongly adsorbed on the surface as LH mechanism or CH₃ radical weakly adsorbed over the active site and OH as ER mechanism. Then the combination between CH₃ and OH on Fe@N4G can occur easily and create methanol compound as a product with low energy barrier both LH and ER mechanisms. The results conclude that the newly developed catalyst (Fe@N4G) is a good candidate for conversion of N₂O and CH₄ gases to the methanol as the valuable compound at mind condition.

Keywords: Methane oxidation; Fe embedded functionalized graphene; LH and ER mechanisms.