Predicting the catalytic activity of transition metal doped TiO_2 for plasma-assisted methane coupling reaction

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Methane supply has been increased with the development of shale gas. The increase in supply has reduced the price and increased the commercial potential of the methane-reforming industry. However, the extreme reaction condition (T > 750 ℃) due to the strong C-H bond is still an obstacle to growth of the methane-reforming industry. The dielectric-barrier-discharge plasma reaction can reduce the reaction temperature of methane coupling. We performed a theoretical study of the catalytic properties of transition metal-doped TiO_2 during the plasma assisted methane coupling reaction. First, the reaction and activation energies of the whole reaction steps were calculated using density functional theory. The reaction and activation energies showed linear relationships with the vacancy formation energy, which is a descriptor of the methane coupling reaction. Second, turn over frequency was calculated using plasma implemented micro-kinetics modeling. In the comparison of plasma on and off, the plasma effect shifted the volcano plot to the left. Our results can provide helpful insight for the development of TiO_2-based catalysts for the plasma-assisted methane coupling reaction.