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Direct partial oxidation of methane via single-site chemistry[1]

ARVIN KAKEKHANI, Stanford University, JENS NORSKOV, Stanford University, SLAC national accelerator laboratory — Methane (CH_4), the cheapest source of hydrocarbons, is a difficult-to-store and hard-to-convert chemical, due to strong and isotropic C-H bonds. Having a selective and efficient method to partially oxidize methane into more useful chemicals including methanol, formaldehyde and alkenes has long been an open challenge for catalysis community. The main challenge is selectivity: if a catalytic material interacts strongly with methane, sufficient to break one C-H bond, it breaks all other bonds of the derivative molecules, as well. This leads to over-oxidization to CO_2. Here using density functional theory (DFT) modelings, we discuss the possibility of using defective (vacancy rich) 2-d materials e.g., MoS_2 to effectively trap single transition metal atoms; thereby, creating a single-site chemistry to enhance the selectivity of methane oxidation process. A single-site chemistry leads to competition between intermediates and products for limited active sites. Our strategy is to use this as an effective means to block unwanted reaction pathways leading to over-oxidization.

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