Mechanism of Oxalic Acid Formation from Acetylene on Pt (111) Surface: A DFT Investigation

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The mechanism of electrochemical synthesis of oxalic acid from acetylene on Pt (111) surface has been comprehensively investigated using first-principles method based on density functional theory (DFT). The calculation results show that CHCH firstly react with OH to form CHCHOH, then, the product takes off hydrogen to form CHCHO. Next, CHCHO oxidize to obtain CHOCHO. During the process of CHOCOOH formation, CHOCHO firstly dehydrogenize to form CHOCO, then, CHOCO interact with OH to produce CHOCOOH. Finally, CHOCOOH dehydrogenize to form COCOOH, after that COCOOH react with OH to get COOHCOOH.

Keywords: Pt (111) surface, acetylene, oxalic acid, mechanism, density functional theory.

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