The mechanism of methanol decomposition by CuO. A theoretical study based on the reaction force and reaction electronic flux analysis

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A theoretical study of methanol decomposition using a model representing the initial step of the reaction CH 3 OH + CuO ? CH 2 O + H 2 O + Cu is presented. Theoretical calculations using B3LYP/6-31 G along with Lanl2DZ pseudopotentials on metallic centers were performed and the results discussed within the framework of the reaction force analysis. It has been found that the reaction takes place following a stepwise mechanism: first, copper reduction (Cu +2 ? Cu +) accompanies the oxygen transposition and then a second reduction takes place (Cu + ? Cu 0) together with a proton transfer that produce formaldehyde and release a water molecule.