

## Alcoxysilanes Production from Silica and Dimethylcarbonate Promoted by Alkali Bases: A DFT Investigation of the Reaction Mechanism

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**Abstract :** Several silicon dioxide sources can react with dimethyl carbonate (DMC) in presence of alkali bases catalysts to ultimately produce tetramethoxysilane (TMOS). Experimental findings suggested that the reaction proceeds through several steps in which the first molecule of DMC is converted to dimethylsilyloxy (DMOS) and  $\text{CO}_2$ . Following the same mechanistic steps, a second molecule of DMC reacts with the DMOS to afford the final product TMOS. Using a cluster model approach, a quantum-mechanical investigation of the first part of the reaction leading to DMOS formation is reported with a twofold purpose: (1) verify the viability of the reaction mechanism proposed on the basis of experimental evidences. (2) compare the behaviors of three different alkali hydroxides MOH, where M=Li, K and Cs, to determine whether diverse ionic radius and charge density can be considered responsible for the observed differences in reactivity. Our findings confirm the observed experimental trend and furnish important information about the effective role of the alkali hydroxides giving an explanation of the different catalytic activity of the three metal cations.

**Keywords :** Alcoxysilanes production, cluster model approach, DFT, DMC conversion

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