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Activation of Light Alkanes on Pure and Fe and Al Doped Silica Clusters: A Density Functional and ONIOM Study

Mehmet Ferdi FELLAH, Işık ÖNAL
Department of Chemical Engineering, Middle East Technical University,
Ankara, 06531-TURKEY
e-mail: ional@metu.edu.tr

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Authors

chem@tubitak.gov.tr

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Abstract: C-H bond activation was studied by use of density functional theory (DFT) and ONIOM calculations as implemented in Gaussian 2003 at the B3LYP level utilising 6-31G* as the basis set for Si, Al, and Fe atoms and 3-21G** as the basis set for O and H atoms. Relative energy profiles were determined for pure silica modeled by a Si_7O_{21} cluster and Fe and Al doped silica clusters via coordinate driving calculations. The activation barriers for C-H bond activation of methane and ethane decrease with the substitution of Fe on the silica surface, which theoretically demonstrates a favorable effect of Fe substitution on that surface. The activation energy barriers of methane and ethane are substantially decreased from the approximate transition state values of 55.14 kcal/mol and 54.89 kcal/mol for pure silica cluster to 33.43 kcal/mol and 36.54 kcal/mol obtained for the approximate transition state for Fe substituted silica, respectively.

Key Words: C-H bond activation, methane, ethane, silica, Fe doping, Al doping, density functional theory, DFT, ONIOM

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