A DFT study to module a SiO2 messoporius surface

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## Abstract

Three -Quartz ,spacegroup 180, surfaces were modelled using crystallographic data from pearson…. obtained in the Medea package database. Surface planes with miller indexes 100, 110 and 200 were cut from the bulk structure. The different surfaces were compared to identify the ideal MCM-41 surface to be used as a Grubbs catalyst support.

## Introduction

The utilisation of homogeneos catalysts in industry are limited, due to the fact that it is expensive to extract the catalyst from post-reaction mixtures (Balcar & Čejka, 2013)(Kotzé, 2015). The use of porious materials as support surfaces for homogeneous catalists became a reality in 1992 with the successful synthesis mesoporous materials. Mesoporous silicates have a periodic structure, although the walls are not crystalline. The original synthesis of mesoporous support material was defined as the M41S family containing hexagonal MCM-41, cubic MCM-48 and lamellar MCM-50 structures. A more visual representation of the different structures can be seen in

Figure 1: Different structures of the M41S family.[9](Izumi *et al.*, 2004)

## Experimental

## Results and discussion

Balcar, H. & Čejka, J. 2013. Mesoporous molecular sieves as advanced supports for olefin metathesis catalysts. *Coordination Chemistry Reviews*. 257(21-22):3107–3124.

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