

## The roles of fluoride in the synthesis of silica zeolites: Periodic quantum chemical studies

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The fluoride-route of synthesis is now crucial to obtain pure silica zeolites. These materials have attracted great interest owing to their actual and potential technological applications that rely on the unique combination of micro-porosity, hydrophobicity and thermal stability they feature. However, the main processes occurring in the directed synthesis of such compounds are still poorly understood. The present talk provides some new insights on this issue by considering recent computational studies performed at the periodic hybrid-DFT level of theory as implemented in the CRYSTAL06 code.