



**Simposio Internacional: Zeoforum: Foro sobre la innovación en zeolitas y materiales porosos ordenados**

***International Symposium: Zeoforum: Forum on innovation in zeolites and ordered porous materials***

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## **Computer Modelling as a Tool in the Science of Microporous Materials**

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Computational modelling is now used widely and routinely in solid state and material chemistry and the application of the techniques to microporous materials has proved to be particularly fruitful. This lecture will aim to review the current state-of-the-art of the field by describing recent progress in the following areas:

- Modelling and prediction of structure
- Simulation of condensation reactions relating to pre-nucleation
- Modelling of active site structures
- Elucidation of reaction mechanisms

Future directions and prospects for the field will also be discussed

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