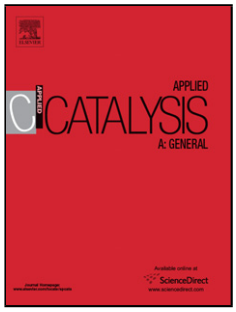

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Ethene hydrogenation on zeolite-supported rhodium clusters. A mechanistic study by density functional and microkinetic modeling

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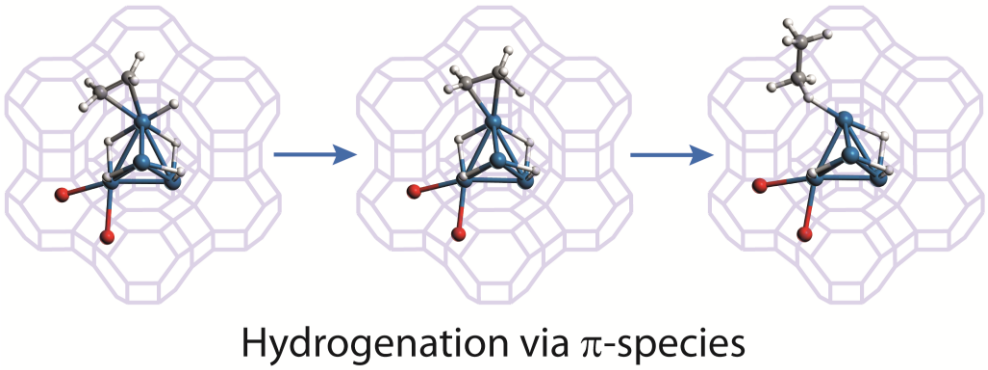
Graphical abstract



Highlights

- Small zeolite-supported metal particles are promising candidates as catalysts in industrial processes.
- The amount of pre-adsorbed hydrogen affects the performance of small Rh particles, anchored in a zeolite, regarding the catalytic hydrogenation of ethene.
- Electronic structure calculations and microkinetic modeling show that π-adsorbed ethene is the active species in the hydrogenation to ethane, just as on TM surfaces.
- The coordination mode of hydrogen on TM clusters is crucial for defining the hydrogenation barriers, e.g. ~30 kJ/mol at high H loading where weakly bound H ligands react more easily.

Abstract

Experiments showed small Rh clusters, supported in zeolites, to be catalytically active in the hydrogenation of ethene. We report a computational study on the transformations of ethene over Rh_4 clusters supported in a faujasite zeolite framework, in particular on the influence of