# CO dissociation on magnetic Fen clusters

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**Résumé**

This work theoretically investigates the CO dissociation on Fen nanoparticules, for n in the range from 1 to 65, focusing on the size dependence in the context of the initial step for the Fischer-Tropsch reaction. CO adsorbs molecularly through its C-end, on a triangular facet of the nanoparticle. Dissociation becomes easier when the cluster size increases. C atom is bonded to a square facet that is generated as a result of the dissociative adsorption, if it does not yet exist in the bare cluster, while the O atom is adsorbed on a triangular facet. Despite the small size of the iron cluster considered, fluctuations due to specific configurations do not influence properties for n> 25 and global trends seem significant. Finally, the use of a support (TiO2-110 facet) can enhance significantly the dissociation energy or make it favorable. The case of study of Fe4 is presented.

**Mots-Clés:** Iron cluster, spin magnetic moment, phase transition

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