Transition Metal Doped Magnetic Zn_iS_i Nanoparticles: i=9,12,16

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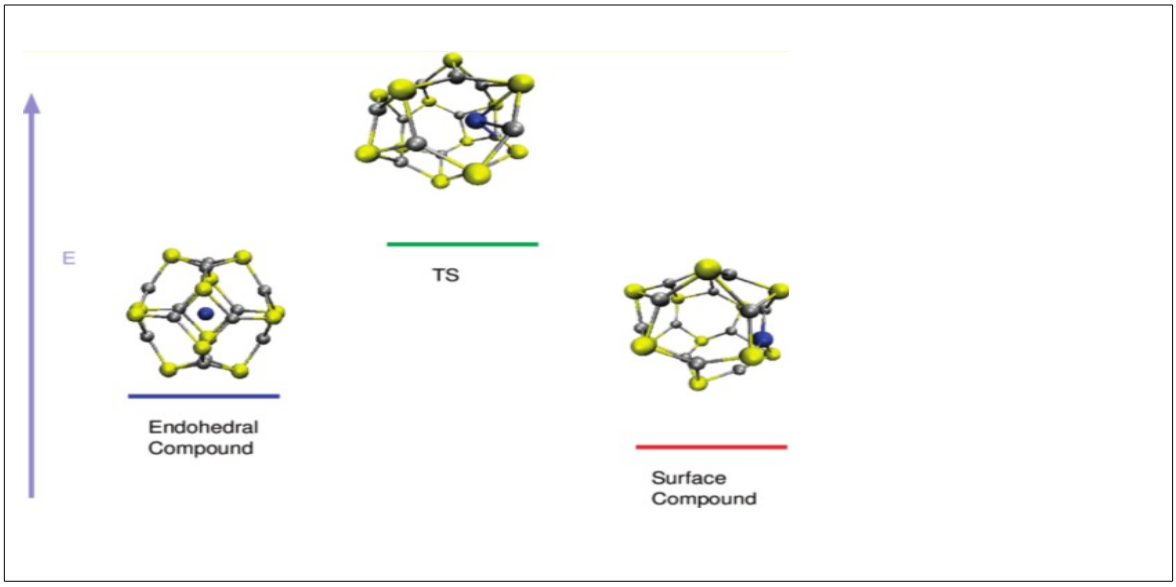
In this work, the endohedral TM@ZniSi have been characterized for i=9,12,16, where TM stands for the first-row transition metals. Their thermodynamic and kinetic stability have been calculated comparing their relative stability with surface structures and the TS's connecting both isomers (see Figure below). Calculations were carried out using DFT functionals taking into account dispersion effects, such as PB3-D3BJ and M06.



In previous works[1,2,3] it was calculated that in general, surface compounds where more stable than endohedral ones. In addition, estimation the lifetimes of the endohedrally doped nanoclusters predicted few to be stable enough. However, in previous works dispersion was not taken into account. In this work we have seen that dispersion effects are very important for endohedral compounds, and therefore the estimation of their lifetimes have been recalculated. Interestingly, endohedral compounds are predicted to be more stable than surface compounds, with long lifetimes.

Bibliography

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