



## College on Multiscale Computational Modeling of Materials for Energy Applications 4 - 15 July 2016

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## Being a "Valentino" at the Nanoscale

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## Abstract:

Morphologies and structural transitions, as well as chemical orderings, play a fundamental role in determing physicochemical properties of nanoclusters, or nanoparticles. We will review what is this 'new' phase of matter, why nanoparticles look so fancy and how we can model them by means of atomistic simulations, with a focus on their catalytic and magnetic properties.