A SURVEY ON THE JOINT USE OF EXPERIMENTAL AND THEORETICAL METHODS AND TECHNIQUES IN MATERIAL SCIENCE

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The presentation will summarize our results on the joint use of experimental and theoretical methods and techniques on some relevant studies on material science. Extensive benchmarks and applications will be presented, covering different fields: i) On the origin of the photolumiscence properties of perovskite based materials. ii) Structural and electronic properties of oxide heterostructures. iii) Phase transitions driven by pressure. iv) Metal intercalation and diffusion processes in solid materials. v) Growth mechanism of pure and mixed metal oxide nanostructures. vi) Formation of conducting zig-zag nanotube like structures from polymers composed of Au_{32} (I_h) units. vii) Development of multifunctional compounds combining conductivity and ferromagnetism behavior.