Quantum confinement in hierarchical self-assembled $CaMoO_4$ nano-octahedron and its photoluminescence property

V. M. Longo,[1,] L. S. Cavalcante,[1] E. C. Paris,[2] J. C. Sczancoski,[2] J. Andrés,[3] E. Longo[1] and J. A. Varela[1]

[1]*LIEC, Instituto de Química, Universidade Estadual Paulista, 14800-900, Araraquara, SP, Brasil*

[2] *LIEC, Departamento de Química, UFSCar, 13560-000, São Carlos, SP, Brasil*

[3]*Departament de Química Física i Analítica, Universitat Jaume I, 12071 Castello, Spain*

The organization of nanomaterials through self-assembly is an important example of the order-disorder evolution of nanoscaled systems. Mesostructured nanocrystals show an impressive ability to self-assemble and self-organize which presents an intriguing challenge to our ability to control and understand order-disorder effects. These self-assembled hierarchical and repetitive superstructures provide promising complex functions[1] and direct bridges between nanoscale objects and the macroscale world. Self-assembly materials are usually highly crystalline and ordered, but surfaces and interfaces play an important role because these materials have disordered transitions regions in the intermediate range order. When the assembly dimensions are in the order of a nano or a few microns, the effects of these disorder regions become considerably more important and lead to surprisingly different properties.

This work, represents a study of the self-assembly process of $CaMoO_4$ (CM) nano-octahedrons obtained by a co-precipitation method and a microwave-hydrothermal system. First-principle calculations have been carried out to model distortions along CM crustal planes (010) and (001) (Fig. 1). Five different supercells were constructed, and calculations were made regarding the modulation of the effect of surface defects in the bulk electronic structure in relation to different dimensions. This study provides a deeper insight into understanding the optical properties derived from quantum confinement and surface defect presented by nano materials. On the experimental side, a number of complementary characterization techniques such as field emission scanning electron microscopy (FEG-SEM), X-ray diffraction (XRD), micro-Raman spectroscopy (MR), optical-absorption (UV-vis) and photoluminescence (PL) spectroscopy were used to obtain a clearer physical picture of the self-assembly $CaMoO_4$ (CM) nano-octahedrons.

Keywords: Sef-assembly; $CaMoO_4$, nano-material, *ab initio* calculations.

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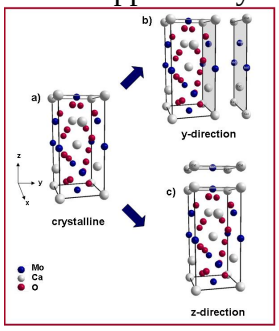

FIG. 1. a) Ordered model of symmetric CM_O; b) asymmetric CM_Y model of (010) plane displacement in the y-direction; c) asymmetric CM_Z model of (001) plane displacement in the z-direction.

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