Strained semiconductor clusters in sodalite

F. Buda[1] and A. Fasolino[2]

[1] *Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands*

[2] *Research Institute for Materials, Institute of Theoretical Physics, University of Nijmegen, Toernooiveld, NL-6525ED Nijmegen, The Netherlands*

We have studied, by the ab initio Car-Parrinello molecular dynamics approach, the structure and band gaps of III-V semiconductor clusters included in sodalite as a function of the cluster size up to full filling of the sodalite cage. This study allows to address directly the role of quantum confinement. The minimum energy structures present large deviations from bulk-like tetrahedral coordination and are reminiscent of amorphous structures. In contrast to the quantum confinement picture, the energy gap grows for increasing cluster size. The shift of the gap is instead due to an effective tensile/compressive strain exerted by the cage on the cluster and is comparable to the variation of the bulk band gap under the effect of hydrostatic pressure.