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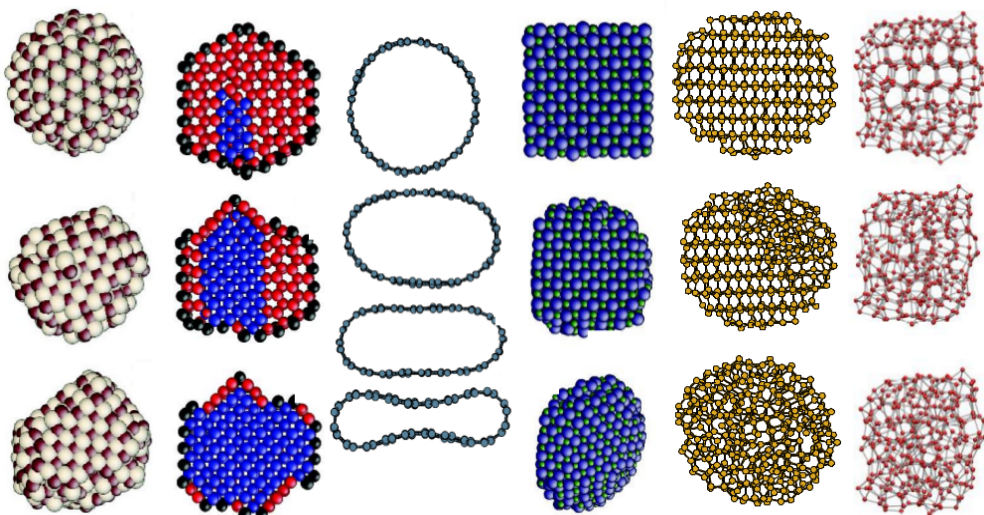
*Department of Physics seminar*  
**DIPARTIMENTO DI FISICA, VIA CELORIA 16, MILANO**  
**Aula Caldirola**  
**April 21<sup>th</sup>, 2017 – 14:30**

## **Order-disorder Interplay and Piezochromic Effects in Nanocrystals under Pressure**

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Nanocrystals show a wealth of distinctive behaviours with respect to their bulk counterparts, which can be tuned by varying their size, shape and surface. These include the way they respond to applied pressure, transforming from the original crystalline structure to new ordered or disordered phases. Of particular technological and fundamental interest are nanocrystals of tetrahedrally coordinated materials, such as Si, Ge, CdSe, CdS and ice, which can be driven by pressure toward highly coordinated crystalline or amorphous phases. We have used density functional theory, molecular dynamics and the enhanced sampling method metadynamics to characterize the mechanisms of structural transformations in these nanocrystals, focussing on the competition between amorphization and crystallization, the effects of an implicit or explicit description of the environment and the emergence of metallic phases. Moreover we have investigated, as a function of size and surface ligands, pressure-induced effects in the electronic and optical properties of nanocrystals, which may be exploited in the development of novel pressure sensors.



Students are  
cordially invited

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