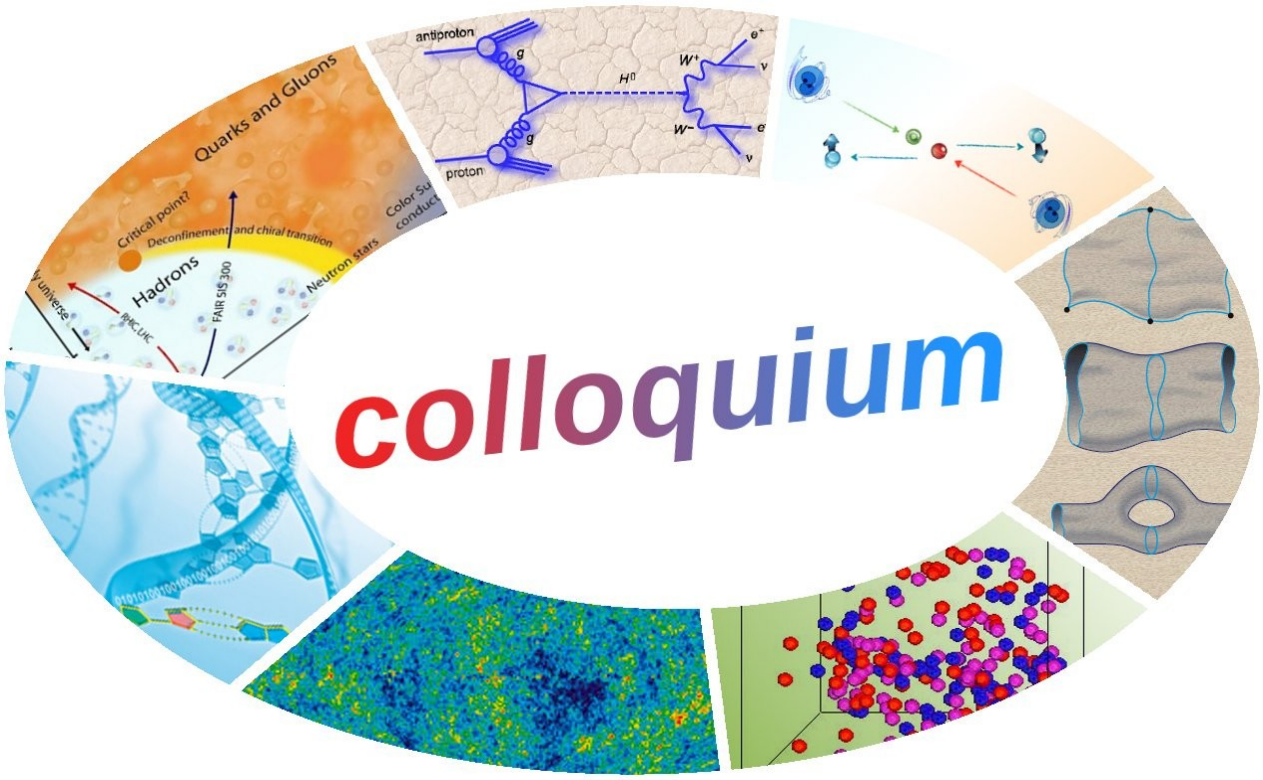
Università di Torino – Dipartimento di Fisica

Sezione di Fisica Teorica



Venerdi 19 Dicembre 2014, ore 14:30, Aula Wataghin

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The quantum mechanical simulation in Materials Science

The pioneering quantum mechanical simulations of solids date back to the years 1975-80. Since then the role of ab initio calculations has been rapidly increasing in many scientific areas and communities, due to decreasing cost of the hardware and availability of computer programs of growing capability and ease of use. The potentialities offered by ab initio simulation techniques in the investigation of the properties of crystalline compounds are illustrated with reference to the CRYSTAL code (www.crystal.unito.it). Basic (the variational basis set, the Hamiltonian, the Density Functional Theory), as well as technical (languages, parallel computing, use of supercomputers) aspects are quickly mentioned. The large variety of crystalline properties that can be evaluated (with various degrees of accuracy), including the elastic, piezoelectric, photoelastic, polarizability tensors, the RAMAN and IR spectra, the equation of state, the effect of pressure and temperature, the charge and momentum distributions, will be illustrated through a few examples.