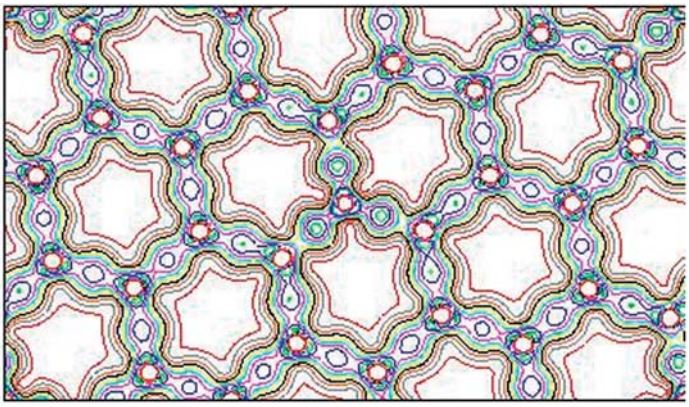
[*C3.* H. Moudden] Effects of Carbon Substitution on Magnesium Diboride : Ab Initio Study

MgB_2 is now widely considered as a non-cuprate high T_c superconductor for which the electron-phonon coupling is unambiguously determined as the main ingredient in the mechanism of its high T_c. But many aspects such as the presence of multi-bands, low concentration of holes and two-dimensionality could be important as well. The C-substitution revealed many new features including the presence of two regimes of T_c depression, and strong enhancement of the critical field. These features are currently under intense research. I made numerical simulations of the C-doping effects [A.H. Moudden, J. Phys. Chem. of Solids 67(2006)115], using super-cells method for high doping, larger than 7% (figure), and recently using the virtual crystal approximation VCA, for doping smaller than 5%. The electronic structure, the Fermi surface, the density of states and the lattice dynamics have been determined carefully within the density functional theory with all electrons and full potentials. Strong electron-phonon coupling could be determined by pseudo-potential codes only. These quantities were then used in the Eliashberg strong coupling approach of superconductivity [G.A. Ummarino et al. Phys. Rev. B.71, 134511(2005)] with some success in describing the C dependence of T_c. The role of inter band scattering and Coulomb screening remain under active investigation.

[Collaboration: A.H. Moudden , LLB,G.A.Ummarino et al. Politecnico di Torino]



Valence electron redistribution near the doped C at the centre:
Hexagonal Super-cell √7x√7

[*C4.* G. Kneller] Relaxation dynamics and quasielastic neutron scattering in proteins from the model of fractional brownian dynamics

The non exponential relaxation in a complex system like a protein can be described by the **fractional brownian dynamics** of a single particle. Such a model describes a protein on a coarse grained scale and localised motions cannot be described within such a model. The fractional brownian dynamics which has absolutely no characteristic time scale is certainly an idealized mathematical model of a physical system which has a very broad but limited distribution of relaxation times. The simulation study that we performed for **lysosyme** revealed a signature of fractional Brownian dynamics in the collective dynamics of the protein. The concept of fractional brownian dynamics leads to the introduction of generalized lorentzians which describe empirically the very broad quasielastic neutron scattering spectrum obtained from internal protein dynamics. The study of the average mean square displacement of the atoms in **lysosyme** has shown that fractional brownian dynamics models may be used to extrapolate the dynamics in a certain way to very long time scales. In this respect these models describe the slow relaxation processes. Thus the extrapolation of the properties of these models in combination with computer simulations can help to study the slow relaxation processes in proteins in particular to establish a signature of protein function.

These type of models we have introduced help to connect the **rapid** dynamics seen by **Quasielastic Neutron Scattering** to the **slow** dynamics more characteristic of the of the protein

[G.Kneller, Phys. Chem. Chem. Phys., 2005, 7, 2641-2655]