Interplay between magnetism and superconductivity near the pressure induced Mott transition in the A15-Cs_3C_{60} compound.

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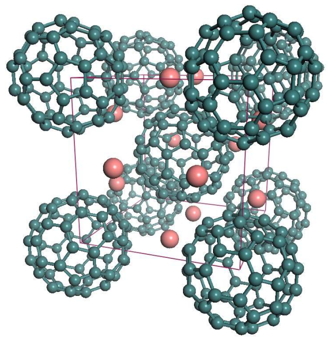
In many families of compounds in which electronic correlations (EC) are of importance, the phase diagrams exhibit magnetic phases proximate with a SC phase. It is often thought that the ECs are at the origin of the superconducting pairing. We have addressed the specific case of the A_3C_{60} compounds, where A is an alkali metal. Initial investigations have led one to consider that a BCS electron-phonon mechanism prevails, with a pairing mediated by on ball optical phonon modes. However further detailed studies of A_3C_{60} compounds gave evidences that their electronic properties cannot be explained by a simple band filling of the C_{60} lowest unoccupied molecular level and it became clear that the influence of ECs generated by Jahn-Teller Distortions (JTD) of the C_{60} balls should play a major role in superconductivity. The debate on this incidence of ECs and JTD, which has been anticipated from DMFT calculations has been reopened by the discovery of two Cs_3C_{60} isomeric phases which present the most expanded lattice in the A_3C_{60} family. Those exhibit an insulator to SC transition with increasing pressure p from a Mott insulator (MI) at ambient p with a dome shaped SC range.

Our NMR experiments under pressure, where p is used as a single control parameter of the C_{60} balls lattice spacing, allowed us to probe the evolution of the SC properties when the ECs are progressively increased toward the MI phase [1]. We have shown that the SC gap increases slightly with decreasing p towards p_0, while T_c decreases on the SC dome, so that upon approaching the Mott transition $2\Delta/k_BT_c$ increases regularly with respect to the BCS value observed in dense A_3C_{60} compounds. A recent detailed NMR study in the vicinity of the Mott transition [2] allowed us to evidence that, in the A15 phase (Fig.1), the insulating AF and the SC phases coexist only in a narrow p range around p_0=5.0 kbar. This establishes the first order and genuine Mott character of the transition. We show that the step like behavior seen on the ^{133}Cs or ^{13}C NMR spin-lattice relaxation rate and on the ^{133}Cs NMR shift when decreasing pressure is the signature of a recovery of the insulating behavior and not a pseudogap like feature. Our data has led us to establish the *(p,T)* phase diagram presented in Fig. 2, with a critical point at p_c~ 7kbar similar to that known for the liquid-vapour transition.

A detailed analysis of the variation of the quadrupole split ^{133}Cs NMR spectrum allowed us to preclude any cell symmetry change at the 3D Mott transition. We anticipate that the slight change of the quadrupole frequency ν_Q detected at the transition can mostly be assigned to a variation of the cubic lattice parameter as occurs due to a small lattice expansion when entering the insulating phase. An important conclusion from this study is that the normal state properties do not exhibit the pseudogap phase which is quite characteristic of the cuprate phase diagram in which the insulator metal transition is controlled by hole doping.

These ensemble of results bring clear evidence that the increasing ECs near the 3D Mott transition are not significantly detrimental to superconductivity. They rather suggest that repulsive electron interactions might even reinforce electron-phonon superconductivity, being then partly responsible for the large Tc values, as proposed by theoretical models taking the ECs as a key ingredient.



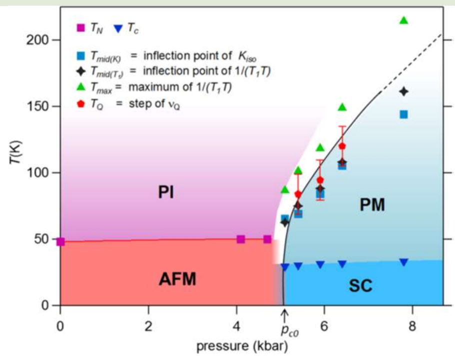


Fig. 1: Unit cell structure of the A15-Cs_3C_{60} phase. Here the body centred cell of C_{60} balls is completed by pairs of Cs atoms lying on the cube faces which are organized in chains in the three lattice directions.
Fig. 2: The (p,T) phase diagram of A15-Cs_3C_{60} displays at low T a narrow first order transition at p_0 between a Néel AF and a SC state. At higher pressures the thermal expansion at fixed p induces a recovery of the insulating paramagnetic state through a transition which broadens with increasing p up to a critical point p_c ~7 kbar. (see PRL **118**, 237601 (2017) for details.

*(1) P. Wzietek, T. Mito, H. Alloul, D. Pontiroli, M. Aramini, and M. Ricc`o; PRL **112**, 066401 (2014).*

*(2) H. Alloul, P. Wzietek, T. Mito, D. Pontiroli, M. Aramini, M. Ricc`o, J.P. Itie, and E. Elkaim, PRL **118**, 237601 (2017).*