Alignment of $N@C_{60}$ and its derivatives in host matrices: the road to develop ordered systems for quantum information processing

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Endohedral fullerenes are remarkable molecules with extraordinary properties. The combination of chemical functionalization of the fullerene cage with engineering of the endohedral species can modify the electronic, optical, as well as chemical and physical properties of the molecule for a variety of applications. Perhaps the most exotic application of them all is the use of endohedral fullerenes as building blocks for an electron-spin-based quantum computer. The two main challenges that need to be addressed are: a) the synthesis of spin-spin coupled endohedral fullerene systems b) the alignment of these systems in a host matrix.

We have achieved good progress in the chemical functionalization of endohedral fullerenes, culminating in the first ever synthesis of a covalently linked $N@C_{60}$-$N@C_{60}$ molecule exhibiting dipolar coupling between the neighbouring electron spins. This is an important milestone. The next one is to engineer ordered structures of endohedral fullerene derivatives.

In this talk, I shall review our efforts in creating ordered fullerene arrays using host matrices such as liquid crystals and polymers. I shall discuss the effect of important molecular parameters such as aspect ratio and functional group rigidity on the degree of fullerene alignment in order to satisfy the orientational requirements for quantum information processing. I shall also discuss the effect of the host matrix on the relaxation properties of $N@C_{60}$, focusing on ways to conserve the long phase memory coherence time of $N@C_{60}$ and its derivatives.