Institut de Química Teòrica i Computacional

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Open-Shell Organic Electronic Materials

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Dimars, 28 de maig de 2013, 15 h
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Semiconducting materials comprised of molecular and polymeric π-conjugated organics have been extensively investigated for a variety of applications in optoelectronic devices such as field-effect transistors (OFETs), light-emitting diodes (OLEDs), and photovoltaic cells (OPVs). The development of "smart" materials in which light or magnetic field is used to modulate the electrical properties of materials is crucial for optical memories and switches, optoelectronics, spintronics, smart surfaces, and bionanodevices.
Toward this end, we have investigated the effect of light and magnetic field on open-shell organic conducting materials consisting of stable delocalized π-radical-based molecules and polymers. A series of spin-delocalized electron-donor radicals, 1,3-diphenyl-benzotriazinyls (BT), and electron-acceptor radicals, benzonitronyl nitroxides (BNN) have been prepared which function as both charge and spin carriers in organic materials. We have found that the electrical conductivities of a majority of our radical systems were much higher (σ_{RT} = 10^{-6}-10^{-2} S cm^{-1}) than typical closed-shell organic compounds, which are typically insulators.