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Understanding of the charge carriers dynamics in poly(p-phenylene) under external electric and magnetic fields. M.R. MAHANI, A. MIRSAKIYEVA, A. DELIN, Department of Materials and Nanophysics, KTH Royal Institute of Technology — Conducting polymers have emerged as highly attractive materials with very diverse applications among which, the charge and spin transport are of central importance. Due to the large electron-phonon coupling in these one-dimensional systems, charge is thought to be transported mainly in the form of polarons, in which trapped charge localizes itself with an associated structural distortion. The dynamics of these charge carriers which carry spin (polarons) are complex and an improved insight into the underlying processes is vital for improving device performance. We address the effect of electric and magnetic fields on the electronic excitations in doped poly(p-phenylene), PPP, using the Su-Schrieffer-Heeger (SSH) tight-binding model. The electric field is included in the Hamiltonian through the time-dependent vector potential via Peierls substitution of the phase factor and magnetic field via Zeeman term. The Zeeman splitting caused by the magnetic field breaks the spin degeneracy of the energy levels. Our calculations reveal three regimes of electric field, based on the charge-phonon coupling, the coupling of charge to acoustic and optical phonons as well as dissociation of the polarons.

M.R. Mahani
Department of Materials and Nanophysics, KTH Royal Institute of Technology

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