ELECTRON SELF-TRAPPING IN ANISOTROPIC TWO-DIMENSIONAL LATTICES: 1. NUMERICAL SIMULATION

L. Brizhik, B. Piette[1], W. J. ZakrzewskI[1]

Bogolyubov Institute for Theoretical Physics,
Nat. Acad. of Sci. of Ukraine
(14b, Metrolohichna Str., 03143 Kyiv, Ukraine)
[1]Department of Mathematical Sciences,
University of Durham
(Durham DH1 3LE, UK)

Self-trapped (spontaneously localized) electron states are numerically investigated in a discrete anisotropic two-dimensional electron-phonon lattice. Such a lattice is used as a model of low-dimensional compounds, in the range of parameters characteristic of materials of the conjugated polymers (polydiacetylenes), for which the account is taken of the interchain interactions. The parametric plot is obtained, which shows the range of numerical values of the intrachain and interchain parameters, for which the ground state of an extra electron (hole or exciton) corresponds to a self-trapped soliton-like extended state, to a localized 'small polaron' state, or to a fully delocalized state.