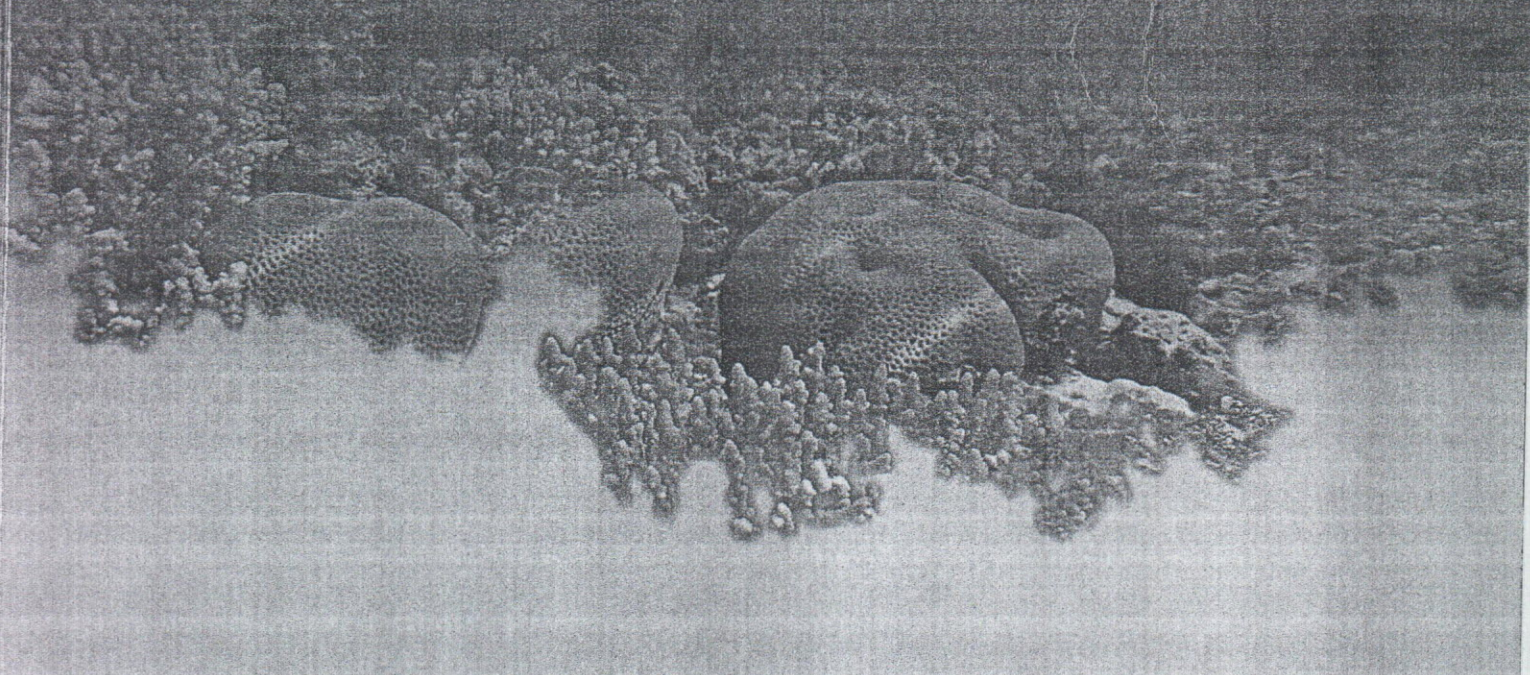# ICSM 2008

International Conference on Science and Technology of Synthetic Metals

Porto de Galinhas Brazil July 6-11, 2008

Book of Abstracts

A NANOCARRRIER CHARGE MODEL FOR THE TRANSPORT IN POLY(O-ALKOXYANILINES)

Fabio de Lima Leite *(USP/Embrapa (Brazil))*, Marcelo Luiz Simões *(Embrapa (Brazil))*, Mário de Oliveira Neto *(USP (Brazil))*, Ranylson Marcello Leal Savedra *(USP (Brazil))*, Paulo Sérgio de Paula Herrmann Junior *(Embrapa (Brazil))*, Igor Polikarpov *(USP (Brazil))*, Ladislau Martin Neto *(Embrapa (Brazil))*, Milan Trsic *(USP (Brazil))*, Luiz Henrique Capparelli Mattoso *(Embrapa (Brazil))*, Osvaldo Novais de Oliveira Junior *(USP (Brazil))*

The mechanisms for charge transport and the nature of the charge species have been controversial. Here we propose a structural model for poly(o-alkoxyanilines), where the conduction process is governed by nanocarriers or quasi-particles with concomitant hopping and tunneling between conducting islands. The metallic islands are coupled into the network with the twisted and tangled polymer chains. We studied the formation of charge carriers in poly(o-alkoxyanilines) using electron paramagnetic resonance (EPR), which shows the presence of two types of charge carriers in poly(o-alkoxyaniline) solutions for an intermediate pH value (pH=5.0). The first type is localized in the amorphous part and with small mobility, while the second is delocalized in the semi-crystalline part with high mobility. Using small-angle X-ray scattering (SAXS) we confirm the existence of quasi-particles in solution, corroborated by ab initio procedures based on simulated annealing (see Fig. 1). The model also indicates that the quasi-particles may jump between defects along the polymer chain providing electronic conduction, which are consistent with molecular modeling results (ab initio and semi-empirical). However, it does not discard the hopping process between neighboring chains.
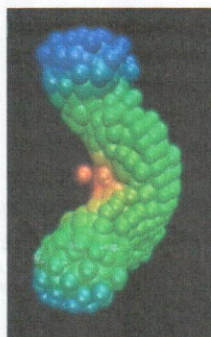
Figure 1. Average Dummy Atom Model (DAM) in pH 3.0 (HCl).