

# Metallomacrocyclic complex bridged polymers: Electronic structures of $-\text{[MacM(L)]}_n$

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The electronic structures of one-dimensional metallomacrocyclics with bidentate bridging ligands, such as  $-\text{[MacM(L)]}_n$  (Mac = phthalocyaninato dianion, tetrabenzoporphyrinato dianion; M = Fe(II), Ru(II), Os(II); L = dabco, pyrazine, triazine, tetrazine (tz), 4,4'-bipyridine, bipyridylacetylene, bis(4-pyridyl)ethylene, bis(4-pyridyl)benzene) have been studied using the tight-binding solid state extended Hückel. The results of this study have shown that the intrinsic semiconductivity properties depend on several factors: (i) the valence band is composed largely of the transition metal dxy orbital; and (ii) the conduction band is composed of a mixture between the macrocycle and bridged orbitals for systems formed by pyrazine, triazine, bipyridine, bipyridylacetylene, etc. However, this composition is different when the ligand tetrazine is used. Such a band is formed by the  $\pi$  system of tetrazine ligand. © 2001 Elsevier Science B.V. All rights reserved.