Nanoscale physics

Electron spectrum of the intercalated stage-ordered layered structures

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Influence of intercalation on the electronic band structure of the layered nanohybrid compound with a stage ordering (three layers in the packet in the considered case) of the GaSe-type is studied in the limiting case of the periodic Anderson model. These materials are promising as cathodes for high-capacity secondary cells and supercapacitors. Intercalated particles form an additional band (usually placed near the initial main band) like the narrow impurity band (being far enough from the main band) or the more extended band hybridized with the main one (for the case of overlapping) (see Fig. 1). The most pronounced transformation of the main band takes place in the vicinity of the impurity level. In the low-temperature limit the frequency dispersion of the density of electron states describes the dependence of the transverse quantum capacity $C_{\perp}(V)$ on the external electric field V.

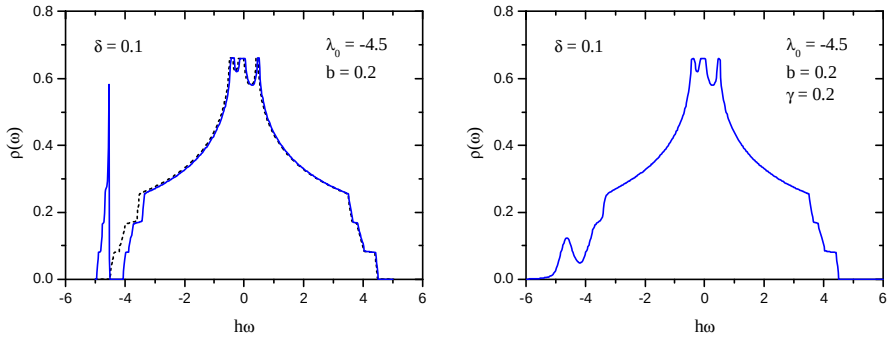

Fig. 1. Density of electron states for the intercalated system in the impurity single-level approximation (left) and the one with the level smearing out (of the Lorenzian-type) due to local electron correlations (right). The dashed line (left) corresponds to the pure matrix. Such model parameters as the site energy difference of the inner and outer layers δ, depth λ_0 and width γ of the impurity level, hybridization energy $b = |V|^2$ as well as interpackage (t = 0.3) and intrapackage (t' = 0.1) electron transfers are given in the units of the interlayer $t_{\perp}$ electron transfer.