CRETE CENTER FOR QUANTUM COMPLEXITY AND NANOTECHNOLOGY

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1st Floor Seminar Room

Adiabatic large polarons in coupled molecular chains

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Abstract

The effects of the lattice discreteness and inter-chain coupling on the properties of the large acoustic polarons in two coupled parallel molecular chains have been studied within the adiabatic approximation. It was demonstrated that the crucial impact on the character of large polarons in such systems has large polaron coupling constant -g. It is defined as a ratio of the lattice deformation energy over the electron bandwidth and its magnitude determines the polaron spatial extent. In the weak coupling limit ($g \ll 1$), when polaron radius highly exceeds lattice constant, we observe the two types of stationary polaron solutions. In particular, for the inter-chain coupling strength below the critical one -$\gamma C \equiv 1/2$, polaron is confined to a single chain. As the coupling between chains increases continual transition towards the delocalization takes place -polaron amplitudes on both chains gradually become equalized, while its binding energy vanishes. Finally, when coupling strength overgrows this critical value, polaron is fully delocalized (symmetric or antisymmetric polaron solution appear) -equally distributed over the both chains, while its energy lies within the band of free states. With the rise of the polaron coupling constant its radius shrinks and lattice discreteness plays important role. In the absence of the inter -chain coupling discreteness manifests itself through the emergence of the bond -centered (*BC*) and site -centered (*SC*) stationary polaron solutions appearing below and above the critical large polaron coupling constant ($gC \sim 0.8727$), respectively. The emergence of these stationary polaron solutions produces the periodic potential, Peierls-Nabarro potential relief, through which polarons have to pass in order to transfer along the chain. It consists of the periodically arranged potential barriers. Below the critical coupling constant these barriers are all positioned at lattice sites, while their heights are all equal. With the increase of coupling strength their positions continuously move away the lattice sites. When polaron coupling constant highly exceeds critical value ($g \gg gc$), all barriers are located at the middle between the adjacent sites. Inter-chain coupling substantially affects the above physical picture. In particular, depending on its strength, we predict the emergence of the asymmetric and symmetric (anti-symmetric), both BC and SC, stationary polaron solutions. Asymmetric solutions correspond to a polaron predominantly distributed over the single chain, while symmetric (antisymmetric) ones corresponds to fully delocalized state equally distributed on both chains. In contrast to weak coupling limit ($g \ll 1$) where the existence of each of these types of solutions is determined solely by the single critical inter{chain coupling constant, here, for each value of g there appear particular critical value of the inter -chain coupling strength -$\gamma c(g)$.