

Abstract Submitted
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Localization and Correlations in Chains of Donors in Si.¹ AMINTOR DUSKO DO AMARAL OLIVEIRA, Physics Institute - UFRJ, ALAIN DELGADO, Department of Physics, uOttawa, ANDRE SARAIVA, Physics Institute - UFRJ, PAWEL HAWRYLAK, Department of Physics, uOttawa, BELITA KOILLER, Physics Institute - UFRJ — Experiments on nanowires of donors in silicon (Si) show metal-insulator transition and ohmic conductance. The understanding of such properties is challenging in view of the expected localization of single-particle electronic states in imperfect 1D systems and many-body localization in strongly interacting 1D systems. We explore disordered nanostructures within a standard single electron approach. Many-body effects are assessed by treating ordered chains. The electronic wavefunction in substitutional P donor nanowires in Si is given as a linear combination of dopant ground state orbitals. The electron-electron (e-e) interactions are included by extending the tunneling Hamiltonian into an extended Hubbard-Kanamori Hamiltonian (HKH). Besides the single particle parameters, on-site energy and nearest-neighbors hopping, the HKH model includes Hubbard (U) and nearest-neighbors direct (V) e-e terms. We compute U and V using the single electron orbitals. Except for U , all parameters depend on relative positions of donor pairs in Si lattice. In the non-interacting regime, disorder leads to electron localization quantified by the localization length. We study the impact of hopping and disorder on observed conductance and the effect of e-e interactions on real space correlations and on absorption of light.

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Amintor Dusko do Amaral Oliveira
Physics Institute - UFRJ

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