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Effect Of Electron Correlation On Shielding Pair Intercation Potential In Carbon Nanotubes JOHN ADAMS, YURIY MALOZOVSKY, Southeastern Louisiana University — We study the effect of short-range and exchange electron correlation in the carbon nanotubes (CNTs). We model the carbon nanotube as a tubule with electrons confined to the surface of the tubule by an attractive delta-function potential. We derived the pair interaction potential between two charges in the presence of the tubule in terms of the generalized random phase approximation (GRPA) incorporating short-range and exchange correlation. The Hubbard like local field factor for the nanotube is derived in terms of the variation procedure of the exchange part of the self-energy for the nanotube with respect to the electron's distribution function. The pair interaction potential is derived for an arbitrary position of two charges with respect to the tubule. We discuss the application of the pair interaction potential for evaluation of the energies of activation for the diffusion of the atomic particles like Li and H in carbon nanotubes. We also discuss application of the pair interaction potential for molecular dynamics simulation of carbon nanotubes.

Yuriy Malozovsky
Southeastern Louisiana University

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