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Theoretical Study of Electron Transport across Carbon Nanotube Junctions Decorated with Au Nanoparticles KHOONGHONG KHOO, JAMES CHELIKOWSKY, University of Texas at Austin — In recent years, there has been extensive research on carbon nanotube networks owing to their potential for applications in transparent electronics, and several experimental studies have found that electrical conductivity across these networks can be increased by metal nanoparticle doping. To aid in understanding the mechanism of this conductance increase, we have performed first-principles calculations on nanotube junctions decorated with small Au nanoparticles. Our calculations show that the conductance of nanotube junctions is significantly increased by the introduction of odd-numbered Au nanoparticles, and electron transport is mediated by resonant tunneling through Au nanoparticle states. In addition, we find that interesting interference effects modulate conduction across doped nanotube junctions that connect near nanotube tips. This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

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