

Abstract Submitted
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TDDFT studies of plasmonic excitations in small transition metal-doped gold chains¹ NEHA NAYYAR, ALAMGIR KABIR, Department of Physics Univ. of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NSTC Univ. of Central Florida — We apply a TDDFT approach to study the absorption spectra of pure Au chains and those doped with transition metal (TM) atoms (Ni, Rh, Fe) up to 24 atoms. We find that for gold chains with more than 10 atoms a collective plasmon mode is formed whose intensity grows with the number of atoms. The plasmon energy approaches asymptotically a value of 0.6eV when the number of atoms is about 20. However, in the chains with odd number of atoms, an additional low-energy excited state close to the plasmonic peak is found which can be related to an excitation at the chain edge. Doping with TM atoms also leads to the formation of additional plasmon peaks close in energy to the main one, especially pronounced in the case of Ni- doped chains. We compare the results for the optical absorption spectrum of the system in the case of doping by different TM atoms and the role of the d-electron states of these atoms in formation of the additional plasmon peaks.

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