

Abstract Submitted  
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**Tunable optical excitations in transition-metal doped arrays of noble-metal chains**<sup>1</sup> NEHA NAYYAR, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando, FL — We apply time-dependent density-functional theory to study the absorption spectrum of arrays of nano-scale pure noble and transition metal (TM) chains. We find that as the number of chains in the noble atom array increases the plasmon peak shifts to higher energies and appears in the visible range for an array of three gold chains, each consisting of more than 10 atoms. We also find collective excitations (plasmons) in arrays of TM chains: a behavior distinct from bulk TM systems. Doping noble metal chains with TM atoms leads to additional plasmon peaks close in energy to the main one for the undoped case. We compare the calculated optical absorption spectrum of the doped chains for several different types of TM atoms at different positions in the chains, and provide rationale for the trends. In the multi-chain case, the response is very sensitive to the position of the doped atoms. We argue that the origin of the additional modes is charge oscillations around the impurity atoms. Finally, we analyze the effect of interaction of excitonic modes created in infinite chains with plasmons in neighboring nanochains, including the possibility of resonance excitations and their trapping by the TM impurity atoms.

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Alamgir Kabir  
University of Central Florida

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