

Engineering optical properties of nanomaterials for solar cell applications

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ABSTRACT

Plasmonic nanostructures are possible candidates for reducing the thickness of the photovoltaic absorber layers. Metallic nanoparticles, for example, could be tailored to couple and trap freely propagating plane waves from the Sun into an absorbing semiconductor thin film, or serve as sub-wavelength antennas in which the plasmonic near-field is coupled to the semiconductor. In each case, they are expected to enhance the efficiency of the solar cell. In this talk, after a brief review of the challenges and opportunities in the rational design of nanomaterials for solar cell application, I will present results of application of the time dependent density functional theory (TDDFT) approach to examine the optical properties of pure Au and Ag chains and those doped with transition metal atoms (Ni,Rh,Fe)¹. Our results indicate that in the case of un-doped chains a collective plasmon mode is formed when the number of atoms is larger than ~ 10 . The plasmon energy approaches asymptotically a value of $\sim 0.6\text{eV}$. In the case of chains with odd number of atoms, an additional low-energy excited state close to the plasmonic peak is found. This state comes from the unfilled bond between the even chain edge and the extra (odd) atom. In the presence of doping, the system acquires one or more local plasmonic excited states close in energy to the extended plasmon peak, which is especially pronounced in the case of Ni-doped chains. I will also discuss the role of the transition metal d-electron states in formation of the local plasmon modes. Additionally, I will present an example of manipulation of the optical properties of organic- and dye-molecule conjugated semiconductor nanoparticles to produce high efficiency visible photoluminescence, using the example of folic acid-conjugated titania and ceria nanoparticles.² Using DFT and TDDFT we find that the strong increase of the photoluminescence can be explained by electronic transitions between the titania surface oxygen vacancy states and the low-energy excited states of the FA/APTMS molecule anchored onto the surface oxygen bridge sites in close proximity to the oxygen vacancies.

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² V. Turkowski, S. Babu, D. Le, M. K. Haldar, A. Wagh, Z. Hu, A. S. Karakoti, A. Kumar, A. J. Gesquiere, B. Law, S. Mallik, T. S. Rahman, M. N. Leuenberger, S. Seal, to be published.