Energy band gap engineering through the surface functionalization of silicon nanocrystals induced by plasma.

[1]Research Center for Photovoltaics, National Institute of Advanced Industrial Science and Technology (AIST), Central 2, Umezono 1-1-1, Tsukuba, 305-8568, JAPAN, [2]Nanotechnology and Advanced Materials Research Institute (NAMRI), University of Ulster, BT37 0QB, Northern Ireland, UK

○Vladimir Švrček[1], Marius Buerkle[1], Mickael Lozac'h[1], Calum McDonald[2], Davide Mariotti[2], Koji Matsubara[1],

E-mail: vladimir.svrcek@aist.go.jp

Quantum dots (QDs) in form of nanocrystals with quantum confinement size (less than the Bohr radius) present an enhanced inverse Auger recombination hence the possibility to trigger multiple excitons generation (MEG). An important effect that might significantly enhance the efficiency of solar cells over >50% is the creation of multiple excitons per incident photon absorbed. Since the MEG effect become efficient under concentrated light it is preferable that QDs have a crystalline structure with a clean surface by avoiding the presence of any organic molecules or surfactants. The silicon nanocrystals (SiNCs) at strong quantum confinement size (<3 nm) have a large surface/bulk ratio which allows the control of optoelectric properties through the surface functionalization. Our studies showed that the surface engineering via surfactant free plasma could be efficient for the functionalization of SiNCs surface resulting in energy band gap tuning. We show that during the plasma processing the SiNCs gradually acquires Si-OH based termination, and that OH surface functionalization follows a Langmuir-like adsorption rate. Our experimental findings are well fitted by first-principles DFT calculations of the SiNCs quasi-band structure. The calculations reproduce the experimentally observed dependence of the wavelengths on the OH coverage and clarify the optical gap behavior. We predicted two sections and conditions where the surface functionalization can be very effective for the band gap engineering and MEG, respectively. Furthermore such surface engineered SiNCs are well dispersed in a colloidal solution, so thin films can also be fabricated by various low cost deposition procedures, including simple one-step solution coating. Finally we demonstrate the impact of surfactant free surface engineering for ultra-thin SiNC film fabrication deposited at different temperatures ranging from room temperature up to 300ºC with high optical transparency, excellent film quality and stability over time.