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Enhanced photoluminescence and structural properties of P-doped ZnO nanostructures prepared using thermal chemical vapor deposition of phosphorus pentoxide

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Vapor phase transport assisted by mixture of ZnO/graphite powders and phosphorus pentoxide via thermal evaporation was used to prepare un-doped and P-doped zinc oxide (ZnO) nanostructures. The structure and morphology were characterized by field emission scanning electron microscopy (FESEM) and X-ray diffraction (XRD).The morphological change in the shape of the nanostructure from nanowire to nanoballs can be observed from the Field Effect Scanning Electron Microscopy (FESEM) images. XRD results indicate that P-doped ZnO nanostructures lost the (002) orientation preference and became randomly oriented. Photoluminescence (PL) properties of un-doped and P-doped ZnO showed significant changes in the optical properties providing evidence for several types of defects such as zinc interstitials (Zni), oxygen interstitials (Oi), zinc vacancy (VZn), singly charged zinc vacancy (VZn-), oxygen vacancy (Vo), singly charged oxygen vacancy (Vo+) and oxygen anti-site defects (OZn) in the grown nanostructures. The P-doped ZnO nanostructures have exhibited shifted PL peaks at near band edge (NBE) and red luminescence compared to the un-doped ZnO. These P-doped ZnO nanostructures have potential application possibilities in gas sensors, solar cells and energy harvesting devices like nanogenerators.

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Nanopatterning on H-terminated Si(111) explained as dynamical equilibrium of the chemical reaction with methanol

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Silicon is by far the most important semiconductor material in themicroelectronic industry, mostly due to the high quality of theSi/SiO_2 interface. Consequently, applications requiring chemical functionalization of Si substrates have focused on molecular grafting of SiO_2 surfaces. Unfortunately, there are practical problems affecting homogeneity and stability of many organic layers grafted on SiO_2, such as silanes and phosphonates, related to polymerization and hydrolysis of Si–O–Si and Si–O–P bonds. These issues have stimulated efforts in grafting functional molecules onoxide-free Si surfaces, mostly with wet chemical processes. Nevertheless, there is a lack of understanding the fundamental reaction mechanism behind the formation of a SAM. In this work we look inside the formation mechanism of methanol reacting with a H-terminated Si(111) surface and find a very surprising result – a nanopattern. The formation of a nanopattern as a result of this wet chemical reaction is surprising if one considers initial random grafting on a surface. Even if next nearest neighbor (NNN) sites were kinetically favorable, adsorption would lead to a disordered arrangement. We confirm this by calculating the kinetic barriers of the reaction of methanol with the H-terminated Si(111) surface by density functional theory (DFT) and implementing these values in a kinetic Monte Carlo (kMC) algorithm. Experimentally, we confirm the decomposition of methanol (FTIR and GCMS) to be an important factor, as it would increasethe chemical potential of H_2. The presence of H_2 initiates desorption of the methoxy groups and thereby leads to a kinetic equilibrium of the reaction of methanol with the H-terminated Si(111) surface. Finally, an input of all relevant values into the kMC algorithm provided a qualitative correct image of the formation mechanism of the nano pattern. This work is of broad interest to the materials community because silicon functionalization is critical for a wide range of applications including nanoelectronics, nanosensors, biomedical applications, energy-absorbing and –storing devices, and even catalysis. In particular, chemical control of atomically smooth Si(111) surfaces is becoming more important as these surfaces are used as templates for both organic and inorganic layered systems.

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