Abstract

A high-performance hydrogen gas sensor has been developed that utilizes a proton affinity of 1,4-diketo-3,6-bis-(4'-pyridyl)-pyrrolo-[3,4-c]-pyrrole (DPPP) known as a red pigment. The present sensor is characterized by a remarkable reduction of electrical resistivity by two orders of magnitude even under 0.05 % H_2. In addition, the device operates at room temperature and is reversible. Furthermore, a variety of ambient gases (such as CH_4, CO, CO_2, NO, SO_2 and water moisture) affects scarcely the sensor performance (*i.e.* less than 0.1 % in resistivity).

The above sensor application is based on the accidental finding of a high proton affinity of the N atom of the pyridyl ring in DPPP. Protonation at the N atom is found to bring about an appreciable color change from vivid red to violet, accompanied by a drastic reduction of the electrical resistivity by five orders of magnitude, as well as the appearance of high photoconductivity. Then, our attention was focused on the utilization of the resisitivity change for H_2 gas sensors, and an attempt was made how to dissociate H_2 molecule into protons and how to measure the change of the electrical resistivity. We have solved these issues by integrating an extremely thin layer of Pd or Pt in interdigital electrodes in combination with a DPPP layer. The device structure is: electrode/Pd/DPPP/electrode.

In parallel, we have also carried out X-ray structure analysis on DPPP as well as its electronic characterization in terms of molecular spectroscopy in single crystals. Structure analysis revealed that there are two crystal phases, one of which is found to be appropriate for H_2 gas sensors because the N atom of the pyridyl ring remains unbonded and is available for protonation; whereas, in the second phase, one of the N atom is blocked due to the formation of NH···N intermolecular hydrogen bonds.