Nano Energy

Volume 88, October 2021, 106241

Tailoring the selectivity of ultralow-power heterojunction gas sensors by noble metal nanoparticle functionalization

10.1016/j.nanoen.2021.106241

Oleg Lupan [a b c d]
Nicolai Ababii [b]
David Santos-Carballal [e]
Maik-Ivo Terasa [a]
Nicolae Magariu [b]
Dario Zappa [f]
Elisabetta Comini [f]
Thierry Pauporté [c]
Leonard Siebert [a]
Franz Faupel [g]
Alexander Vahl [g]
Sandra Hansen [a]
Nora H.de Leeuw [e h]
Rainer Adelung [a]

[a] Functional Nanomaterials, Faculty of Engineering, Institute for Materials Science, Kiel University, Kaiserstr. 2, D-24143 Kiel, Germany

[b] Center for Nanotechnology and Nanosensors, Department of Microelectronics and Biomedical Engineering, Technical University of Moldova, 168 Stefan cel Mare Av., MD-2004 Chisinau, Republic of Moldova

[c] PSL Université, Institut de Recherche de Chimie Paris-IRCP, Chimie ParisTech, rue Pierre et Marie Curie 11, 75231 Paris Cedex 05, France

[d] Department of Physics, University of Central Florida, Orlando, FL 32816-2385, USA

[e] School of Chemistry, University of Leeds, Leeds LS2 9JT, United Kingdom

[f] Sensor Laboratory, Department of Information Engineering (DII), University of Brescia, Via Branze 38, Brescia 25123, Italy

[g] Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Kaiserstr. 2, D-24143 Kiel, Germany

[h] Department of Earth Sciences, Utrecht University, Princetonplein 8 A, 3584 CD Utrecht, The Netherlands

Abstract

Heterojunctions are used in solar cells and optoelectronics applications owing to their excellent electrical and structural properties. Recently, these energy-efficient systems have

also been employed as sensors to distinguish between individual gases within mixtures. Through a simple and versatile functionalization approach using noble metal nanoparticles, the sensing properties of heterojunctions can be controlled at the nanoscopic scale. This work reports the nanoparticle surface functionalization of TiO_2/CuO/Cu_2O mixed oxide heterostructures, where the gas sensing selectivity of the material is tuned to achieve versatile sensors with ultra-low power consumption. Functionalization with Ag or AgPt-nanoclusters (5–15 nm diameter), changed the selectivity from ethanol to butanol vapour, whereas Pd-nanocluster functionalization shifts the selectivity from the alcohols to hydrogen. The fabricated sensors show excellent low power consumption below 1 nW. To gain insight into the selectivity mechanism, density functional theory (DFT) calculations have been carried out to simulate the adsorption of H_2, C_2H_5OH and n-C_4H_9OH at the noble metal nanoparticle decorated ternary heterostructure interface. These calculations also show a decrease in the work function by ~2.6 eV with respect to the pristine ternary heterojunctions. This work lays the foundation for the production of a highly versatile array of sensors of ultra-low power consumption with applications for the detection of individual gases in a mixture.