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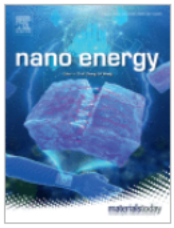

Al_2O_3/ZnO composite-based sensors for battery safety applications: An experimental and theoretical investigation

David Santos-Carballal, Oleg Lupan, Nicolae Magariu, Nicolai Ababii, Helge Krüger, Mani Teja Bodduluri, Nora H. de Leeuw, Sandra Hansen, Rainer Adelung

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Abstract

Lithium-ion batteries are vital in one of the key nanotechnologies required for the transition to a carbon-free society. As such, they are under constant investigation to improve their performance in terms of energy and power densities. At the same time, safety monitoring is crucial, as defects in the battery cell can lead to serious safety risks such as fires and explosions as a result of the enormous heat generated in the electrolyte, causing the release of toxic and flammable gases in the so-called thermal runaway. Therefore, early and rapid detection of the gases that form before thermal runaway is of particular interest. To this end, solid-state sensors based on new heterostructured materials have gained interest owing to their high stability and versatility when used in the harsh battery environment. In this work, heterostructures based on semiconductor oxides are employed as sensors for typical components of battery electrolytes and their decomposition products. The sensors showed a significant response to vapors produced by battery solvents or degassing products, making them perfect candidates for the development of successful new prototypes for safety monitoring. Here, we have used a simple and versatile method to fabricate the Al_2O_3/ZnO heterostructure, consisting of atomic layer deposition (ALD) and thermal annealing steps. These Al_2O_3/ZnO heterostructures have shown a response to the vapours of 1,3-dioxolane (DOL, $C_3H_6O_2$), 1,2-dimethoxyethane (DME, $C_4H_{10}O_2$), $LiPF_6$, ethylene carbonate (EC)

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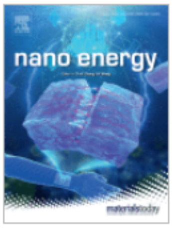

and dimethyl carbonate (DMC), which are typically used as components of the electrolytes in LIBs. The sensors showed a significant response to vapors produced by battery solvents or degassing products, significantly increasing the chances of developing new successful prototypes for safety monitoring. Density functional theory (DFT) calculations were employed to systematically compare the surface reactivity of the α-$Al_2O_3(0001)$ and the $ZnO10\bar{1}0$ facets, as well as the $Al_2O_3/ZnO10\bar{1}0$ interface, towards $C_3H_6O_2$, $C_4H_{10}O_2$, nitrogen dioxide (NO_2) and phosphorous pentafluoride (PF_5), in addition to H_2O to assess the impact of relative humidity on the performance of the gas detector. The scanning tunnelling microscopy (STM) images and molecular binding energies compare well with our experiments. The energies of molecular adsorption at the heterostructure suggest that humidity will not affect the detection of the volatile organic compounds. The results presented here show that the potential to detect vapors of the components used in the electrolytes of LIBs, combined with the size control provided by the synthesis method, makes these heterostructures extremely attractive in devices to monitor battery safety.

Keywords: heterojunctions, battery safety, gas sensing

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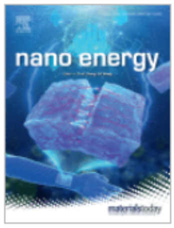

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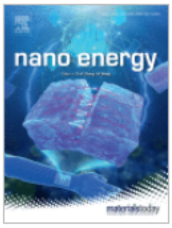

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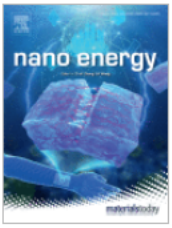
Nano Energy
Volume 109, May 2023, 108301



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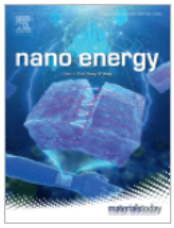

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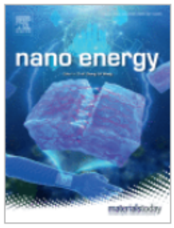

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