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## Heterostructure-based devices with enhanced humidity stability for H<sub>2</sub> gas sensing applications in breath tests and portable batteries

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### Abstract

Semiconducting metal oxide - based gas sensors exhibit outstanding sensitivity, although humidity in the analyte typically hampers precise measurements. In this work it was shown that a 5–6 nm thin Al<sub>2</sub>O<sub>3</sub> nano-layer is particularly beneficial in reducing the interference due to humidity of p-type conductivity copper oxide-based gas sensors. An effective approach from chemical solutions at 75 °C and thermal annealing at 600 °C was used to grow copper oxide nano-crystallite layers. The Al<sub>2</sub>O<sub>3</sub> nano-layers were subsequently

deposited on top of copper oxide by atomic layer deposition in a high-aspect-ratio regime at 75 °C. The morphological, structural, chemical, vibrational, electronical and sensor characteristics of the heterostructured nano-crystallite layers have been studied. The final nano-Al<sub>2</sub>O<sub>3</sub>/CuO heterostructure showed an increase in the response to H<sub>2</sub> gas by 140 %, while long-term stability at low and high relative humidity was observed. The initial sensing response varied by only 10 % for an Al<sub>2</sub>O<sub>3</sub> layer of 5–6 nm on top of CuO with a post-thermal annealing at 600 °C acting as an effective barrier for water vapor and oxygen. A comparison with CuO nanocrystallite layers covered by ALD with 6 nm and 15 nm of Al<sub>2</sub>O<sub>3</sub> ultra-thin films on top demonstrates an exceptional stability of the hydrogen gas response at high relative humidity (84 % RH). Density functional theory-based calculations showed that the H<sub>2</sub> molecule spontaneously dissociates over the formed Al<sub>2</sub>O<sub>3</sub>/CuO heterostructure, interacting strongly with the surface Al atoms, showing different behavior compared to the pristine CuO (111) surface, where H<sub>2</sub> gas molecules are known to form water over the surface. The present study demonstrates that a thorough optimization of technology and surface properties due to coverage and formation of heterostructured nano-materials improves the humidity stability during H<sub>2</sub> gas sensing applications which is important for real-world applications, e.g. portable battery analysis, H<sub>2</sub> breath tests, along with environmental, medicine, security, and food safety diagnostic tests.