Toward selective detection of H₂S gas by AuNPfunctionalized carbyne-enriched based sensors

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Over the past decades, carbon-based nanomaterials have been intensively studied for their application in gas sensing technologies due to their special mechanical and electrical properties.¹ However, most attention has been given to sp²-hybrydized carbon allotropes such as nanotubes (CNTs) and graphene leaving others like carbyne significantly unexplored.

Carbyne is a one-dimensional carbon allotrope with sp¹-hybridization that was predicted in the 1960s having two existing forms; polyyne, which contains alternating triple and single bonds, and cumulene, composed of successive double bonds. This material has been predicted to have novel properties like extreme tensile stiffness, functional tunable mechanical properties and a larger specific strength compared to that of diamond. ^{2,3} Although their synthesis and stability have been controversial over the years, some of these special features have just recently been exploited for the fabrication of gas sensing devices with only two reports published since 2020. First, Yang and coworkers reported the detection of 2 ppm NO₂ gas at room temperature using carbyne nanocrystals (CNC).⁴ Then, Aleksandrova *et. al.* demonstrated the detection of ppm ethanol concentrations using surface acoustic waves-based (SAW) devices coated with carbyne-enriched films.⁵ These results indicate not only the great potential of carbyne as the active material for emerging gas-sensing technologies but also the need for further research in this developing field.

In this context, we present, for the first time, the selective detection of low concentrations of H_2S gas using a chemiresistive multichannel sensing device based on carbyne-enriched films functionalized with gold nanoparticles (AuNP). The device consists of 64 sensors addressed individually by a multiplexing system. The interdigitated electrodes (IDEs) were fabricated using standard UV-lithography and metal deposition methods on polyimide (Kapton) flexible substrates. The carbyne-enriched films were selectively deposited on the IDEs by ion-assisted pulse-plasma deposition (Figure 1a). The films were then functionalized with gold nanoparticles (AuNP) by a potentiostatic electrodeposition technique successfully tested before in other carbon allotropes.⁶ It was observed that increased applied voltages and deposition times resulted in a higher density of AuNP on the films (Figures 1b-1e). The multichannel device was exposed to 500 parts per billion (ppb) of H_2S using N_2 as carrier gas at room temperature showing an increased sensing response ($\Delta R/R_0$) of almost 30% for sensors functionalized with a dense amount of AuNP compared to unfunctionalized sensors (Figure 1f).



These results demonstrate the enhanced selectivity toward H_2S gas by exploiting the strong chemical affinity of sulfur and gold. Moreover, the detection of low ppb concentrations suggests the potential implementation of these sensors in fields like exhaled breath analysis where extreme sensitivity and selectivity are key.

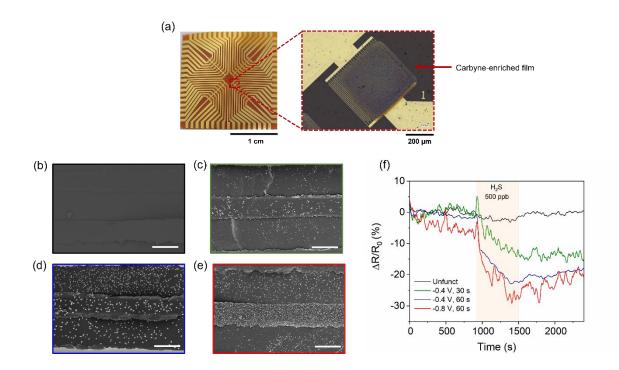


Figure 1. Gas sensing device based on AuNP-functionalized carbyne-enriched film. (a) Photograph of the flexible multichannel sensor and carbyne-enriched film deposited on the IDE. Scanning electron microscopy images of (b) unfunctionalized and AuNP functionalized carbyne-enriched film for (c) 30 s and (d) 60 s at -0.4 V and (e) -0.8 V for 60 s. (scale bar: 5 μ m) (f) Sensing response measured as change of resistance (Δ R/R₀) of unfunctionalized and AuNP-functionalized and AuNP-functionalized and AuNP-functionalized sensors to 500 ppb H₂S at room temperature.

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