High Selectivity of Penta-$BeAs_2$ for Toxic Gas Sensor: A Theoretical Investigation.

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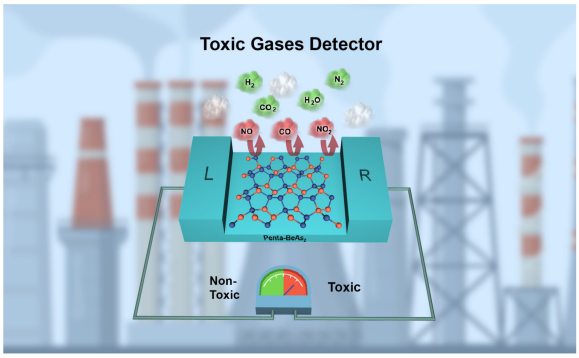
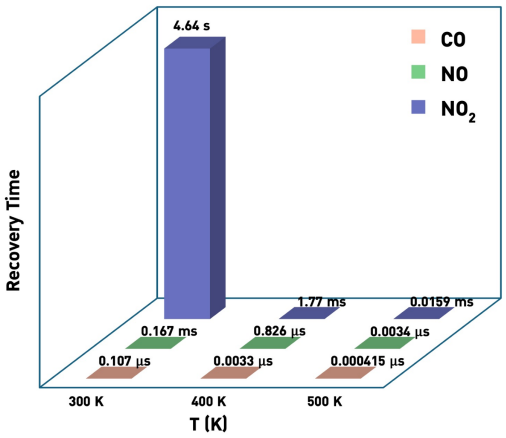
Toxic gases, such as CO, NO, and NO_2, remain a critical challenge for public health and industrial safety. To detect toxic gas, the developing novel two-dimensional (2D) materials with high selectivity and sensitivity is essential. Building on recent studies of the 2D material penta-BeP_2,[1] herein, we theoretically propose penta-$BeAs_2$ as a new member of the pentagon-based family with high selectivity and sensitivity of toxic gas.[2] The adsorption energies of non-toxic gases (H_2, N_2, and CO_2) were distinct from toxic gases (CO, NO, and NO_2), indicating high selectivity. In practice, the adsorption energies of the toxic gas should be in the moderate range between -0.4 and -1.0 eV, resulting in a short recovery time. Recovery time analysis confirms rapid desorption at 300 K, demonstrating its suitability for real-time gas sensing. Additionally, quantum transport properties, studied using the non-equilibrium Green's function (NEGF) approach, confirm strong sensitivity and selectivity toward toxic gases. These findings highlight penta-$BeAs_2$ as a promising material for environmental monitoring and industrial applications.





References

1. Jiang, X.; Wang, Y.; Li, Z.; Zhang, J.; Liu, H.; Wu, D. *ACS Appl. Mater. Interfaces*, **2022**, 35229 – 35236.
2. Sringamprom, S.; Thanasarnsurapong, T.; Watcharatharapong, T.; Hirunpinyopas, W.; Sirisaksoontorn, W.; Prasongkit, J.; & Boonchun, A.; *ACS Applied Materials & Interfaces*, **2024,** 56387-56395.