

FROM SENSING TO MAKING SENSE

A Chemically Programmable Nano-electronic Nose For Multi-threat Detection

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New detectors are urgently needed for the warfighter that provide high specificity, minimal false alarms, wide deployability (e.g., lightweight, low power), and tunable responses to expand the library of detectable threats, eventually including those yet to emerge. To address this need, our team is developing a chemical gas detector based on smart molecular logic encoded in a collection of nanoelectronic sensors on a silicon chip using scalable semiconductor processes. In this presentation, we will describe our LLNL patent-pending technology^{1,2} toward highly specific electronic nose (“e-nose”) chemical sensors with single-digit ppm detection limits and

We used theory-augmented informatics to screen the vast physicochemical property space of thousands of ionic liquid candidates³ to encode highly orthogonal responses across our CNT pixel array. This enables us to chemically program the specificity of our sensor array to various gaseous and volatile threat signatures – e.g., toxic industrial chemicals (TICs) or chemical warfare agents (CWAs). We validated our approach by using 6 functionalized pixels to successfully discriminate 50-ppm levels of ammonia, carbon monoxide, and oxygen over a nitrogen background with high fidelity using a random forest model on training data.

Future work will use LLNL proprietary methods based on Gaussian processes to efficiently analyze large, multi-dimensional training data sets.⁴ As we continue to expand the number of pixels on a chip, our informatics-based screening will aid the programming of more complex ionic liquid assays to enhance the degree of orthogonality in sensor responses. This will allow our detector technology to adaptably identify and quantify diverse threats and at increasingly lower concentrations and faster response times.

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4. Muyskens, A. L.; et al. *The Astronomical Journal* 2022, 163 (4), 148. DOI: 10.3847/1538-3881/ac4e93.

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