A Machine Learning Chemical Classifier using a Bound-State-in-the-Continuum Dielectric Metasurface Filter Array

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The detection and quantification of gases at low concentrations is important to many industrial safety and environmental monitoring settings. These measurements are traditionally performed using Fourier transform infrared spectrometers, which are considered too large and bulky for many applications. Here, we design and simulate an IR microspectrometer (Fig. 1a) based on an array of spectral filters used with a detector array. The spectral filters are dielectric grating metasurfaces that exhibit symmetry-protected bound-state-in-the-continuum (BIC) resonances [1]. We design a set of 16 bandpass filters that span the 3-3.5 um mid-IR band, where short chain acyclic hydrocarbon gases are spectrally distinguishable. We employ a machine learning classifier (MLC), trained on photoresponses produced in our simulated system (including noise) when subjected to five gases (acetylene, ethane, methane, ethylene, and propane). We validate the classifier (see e.g. [2]) by subjecting it to the gases at concentrations from 50 ppm to 5×10^5 ppm, eliciting a mean classification accuracy of 96.4% across all classes and concentrations.

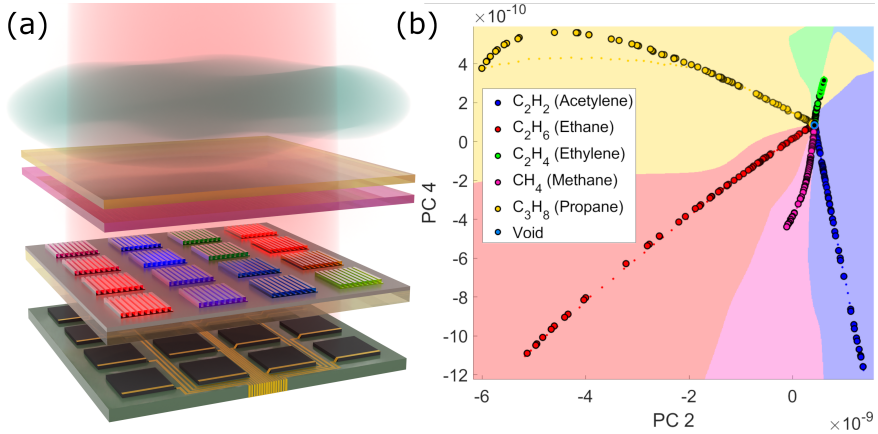

Figure 1: (a) Exploded-view of the simulated microspectrometer system depicting (from top to bottom) the contaminant gas cloud, polarizer, bandpass filter, metasurface array and photodetector array when illuminated by an IR source. (b) 2D Principal component space representations of simulated photodetector array signals with decision boundaries generated by the MLC

[1] J. M. Foley and J. D. Phillips, *Opt. Lett.* **40**, pp.2637-2640 (2015)

[2] J. Meng, J.J. Cadusch, K.B. Crozier. *ACS Phot.* **8** pp.648–657 (2021)