# Biocompatible polymer/perovskite nanocrystals composites for sensing applications

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## Abstract

**In this work, we have developed a photoluminescent chemosensor based on a Molecularly Imprinted Polymer nanocomposite of CsPbBr3 PVKs embedded in a polymer for the selective detection of explosive or explosive-like molecules. The sensor is based on homogeneous and transparent thin films of CsPbBr3 PVKs embedded in polycaprolactone (PCL) as a polymer host matrix and 3-NT as a template. The sensor fabrication is performed by spin-coating. We evaluate the sensing capability of the nanocomposites by exposing the patterns to vapours of some high explosive or explosive-like molecules. Additionally, two different molecules such as 2-mercaptoethanol (MET) and ethylenediamine (EDA) are also tested for comparison. The change in intensity and response times for PCL-PVK MIP and NIP nanocomposites are quite varied depending upon the analyte to which it is exposed. The sensitivity of the sensor was improved by using the PCL-PVK MIP sensor.**

## Background

**Chemical sensors** based on metal halide perovskites have attracted intense interest because of their excellent optical electronic, high absorption coefficients, high quantum emission efficiencies, tunable properties, and solution processability properties [1].

**The sensing mechanism** of the $CsPbBr_3$ PVK sensor is based on the changes of the chemical composition of their environment. Possible sensing mechanisms include doping, gas-induced defect reparation, trap passivation and, ion-exchange [2].

**Analyte interaction on PVK surface → Changes in the emission intensity**

## Sensor Fabrication

### Ex-Situ Synthesis of PVK-PCL Sensor

- 14% Coloidal solution of $CsPbBr_3$ PVK
- 75% Polycaprolactone solution
- 11% o-Xylene extra solvent

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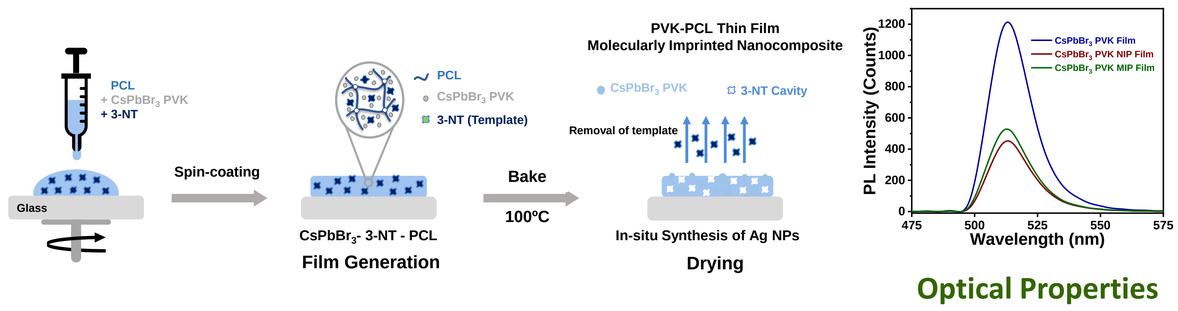
- 80% Resulting Solution
- 20 % 3-NT 8,35 M (MIP) or 20 % o-Xylene (NIP)

### Spin-Coating Miniaturization

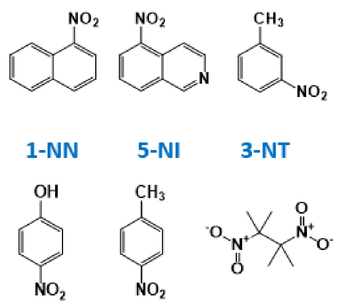



**Optical Properties**

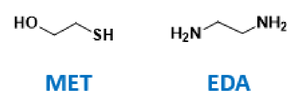
## Sensing Performance

### Analytes of Interest

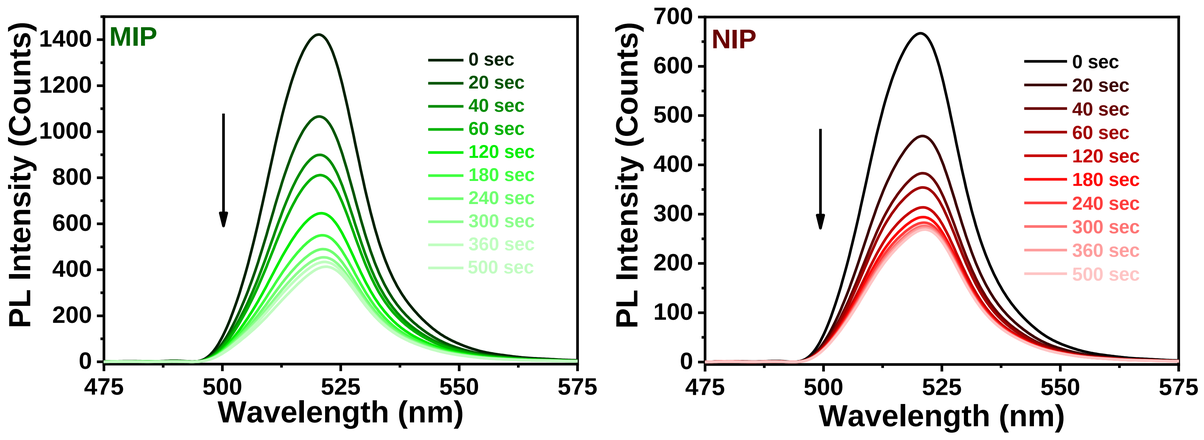
· **Explosive and Analogues**




· **Volatile Organic Compounds**

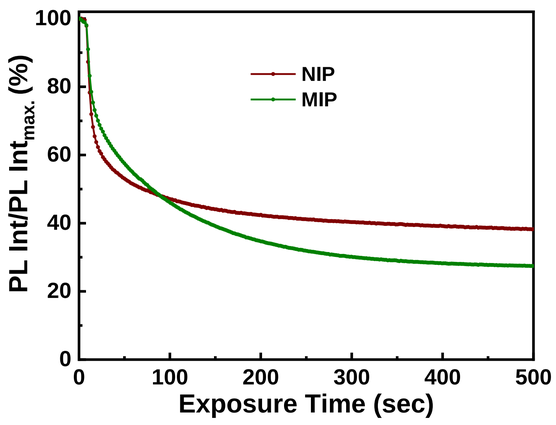



### Exposure to 3-Nitrotoluene

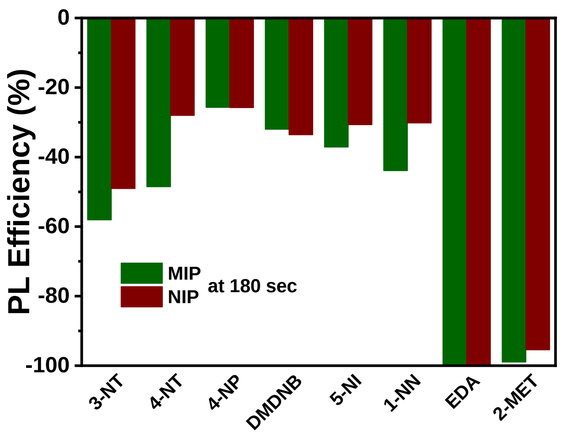



**PL Intensity is very sensitive to the adsoption of $NO_2$-Compounds at $CsPbBr_3$ PVK**

### Real Time Kinetic Response



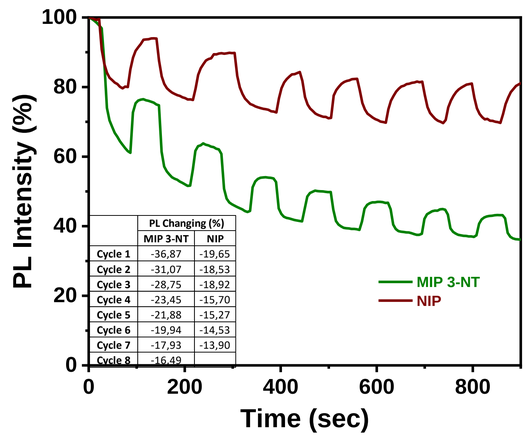

### Exposure to Analytes of interest




| Analyte | PL Eff.$_{MIP}$ (%) | PL Eff.$_{NIP}$ (%) |
|---|---|---|
| 3-NT | -58,05 | -49,04 |
| 4-NT | -48,52 | -28,02 |
| 4-NP | -25,72 | -25,76 |
| DMDNB | -32,00 | -33,56 |
| 5-NI | -37,12 | -30,69 |
| 1-NN | -43,89 | -30,18 |
| EDA | -99,77 | -99,76 |
| 2-MET | -98,94 | -95,44 |

**The chip sensor approach exhibits very fast response (few seconds) and selectivity for nitro-containing compounds**

### Reusable sensor




**The analyte adsorption on the sensor surface is a reversible process**

## Conclusions

· **This nanocomposite can form the basis of a low cost, easy-to-fabricate and portable sensing platform technology for chemo-sensing.**

· **$CsPbBr_3$ nanocomposite showed chemo-sensing performance with very short response times and high selectivity.**

· **PCL-PVK MIP sensor contributes to increase the sensitivity.**

· **Reversible explosive adsorption process allows to reuse the MIP/NIP sensor.**

## References

[1] E. Kymakis, A. Panagiotopoulos, M. M. Stylianakis and K. Petridis, 2D Nanomaterials for Energy Applications, 2020, 131-147

[2] Z. Zhu, Q. Sun, Z. Zhang, J. Die, G. Xing, S. Li, X. Huang and W. Huang, J. Mater. Chem C, 2018, 6, 10121-10137

## Aknowlegments

NATO Project SPS G5361