

# Near Ambient Pressure XPS study of NPG-analyte interaction

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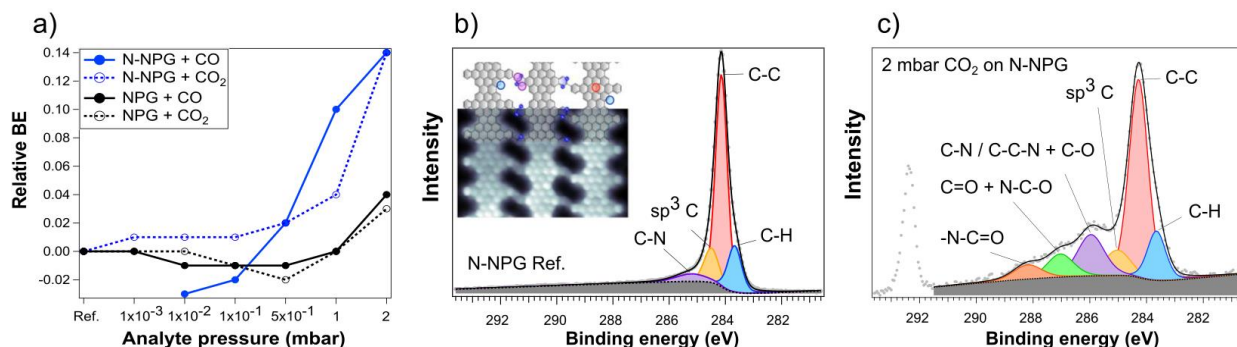
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2D materials are great candidates to overcome the demand of low-power, portable and ultra-sensitive gas sensors. More specifically, graphene is very attractive for this application as its electronic properties can be easily modulated by the interaction with the gas analytes. However, its semimetallic character limits its use in high-sensitive sensors based on field-effect transistors (FET). Likewise, its inertness limits the selectivity, a crucial figure of merit of sensors. In the presented work, we explore the possibility to use atomically precise, undoped [1] and nitrogen doped [2] nanoporous graphene (NPG and N-NPG, respectively) as gas sensors. Both NPGs exhibit a  $\sim 2$  eV semiconducting gap, convenient for FET applications. Their nanopore superlattice can also provide the reactivity needed for sensing applications. Near Ambient Pressure XPS was used to explore in-situ the evolution of chemical interactions and atomic structure during exposition to CO and CO<sub>2</sub>, selected as donor and acceptor analyte models. The gas-analyte interaction results in new components and their overall shift, altogether indicating chemisorption and doping effects (Figure 1a, c). Interestingly, both the relative weight of new components and energy shift are more pronounced for N-NPG, and more subtle differences can be observed for the case of each analyte. Finally, the recovery of XPS features of the pristine samples after an in-vacuum post-annealing indicates a reversible sensor-analyte interaction.

## References

- [1] C. Moreno et al., Science, 6385 (2018) 199-203
- [2] M. Tenorio et al., Adv. Mater., 20 (2022) 2110099

## Figures



**Figure 1:** a) C1s binding energy (BE) shift vs analyte pressure. b) and c) C1s components of the N-NPG reference and at 2 mbar of CO<sub>2</sub>, respectively