

## **In-silico protocol to design plasmonic nanosensors**

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Plasmonic sensors may exploit the huge enhancement of the Raman signal when a molecular system is adsorbed on a plasmonic nanostructured material. The resulting technique (Surface- Enhanced Raman Spectroscopy – SERS) permits single molecule detection, thanks to a specific engineering of the plasmonic material combined with the target molecular system. However, the morphology of the molecule-plasmonic system which gives the best resolution is not known a priori. In this contribution, we present a novel computational protocol which can assist the design a nanostructured plasmonic sensor. Our approach can identify the ideal chemical nature of the plasmonic substrate, its macroscopic and microscopic morphology, the best geometrical arrangement of the couple analyte/substrate, which give single molecule sensitivity. Remarkably, the approach is able to describe at the same level of accuracy any kind of plasmonic materials, ranging from noble metal nanoparticles to graphene-based nanomaterials. The robustness and reliability of the in-silico protocol is demonstrated for selected test cases.