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Project title: Evaluation and application of a semi-analytic solution for the nanoparticle-on-mirror plasmonic construct

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## PROJECT DESCRIPTION:

The plasmonic nanoparticle-on-mirror (NPoM) geometry is one of the most widely used in nano-optics in recent years [1]. Small metallic nanoparticles (NPs), that sustain collective oscillations of their free electrons (plasmons) are brought to interact with their mirror image in an underlying metallic film. To separate the two, thin spacers are used; these can be either simple dielectrics with no interesting optical characteristics (at the wavelengths of interest) of their own, or they can be layers of organic molecules that create conducting paths between the two metals [2], two-dimensional (2D) materials with optical resonances due to the collective excitation of electron-hole pairs (excitons) [3], or even organic "pockets" that carry quantum emitters [4]. This geometry allows thus the design of a richness of nano-optical applications, including material characterisation, molecular optomechanics, and possibly single-photon emission, while the intense and localised electromagnetic field in the NPoM cavity enables enhanced molecular sensing, fluorescence, and Raman scattering. Nevertheless, the combination of a small metallic NP with diameter of just a few tens of nm with a semi-infinite metallic film and an ultrathin (Angstrom-to-nm) spacer makes numerical treatment of this geometry rather challenging. To deal with this problem, our group, in collaboration with KU Leuven, developed recently a semi-analytical method based on spherical- and planewave expansions, as appropriate for each part of the geometry, which are then combined through appropriate transfer and scattering matrices [5].



The aim of this project is to verify, test, and utilise the computational tool developed in [5]. The code is written in **Matlab**, knowledge and experience with which is a prerequisite for the project. The student will first study and understand the basics of the method. Subsequently, examples of increasing complexity and computational cost will be selected, and evaluated in terms of computational time, convergence, and the underlying physics. If time allows it, and the student already has some experience with it, comparison with a commercial finite-element method (**Comsol**) will also be performed, focusing on both the far-field scattering properties of the system and on the near-field enhancement that the NPoM cavity provides.

- [1] J. J. Baumberg et al. Nat. Mat. 18, 668 (2019).
- [2] F. Benz et al. Nano Lett. 15, 669 (2015).
- [3] M. Geisler et al. ACS Photonics 6, 994 (2019).
- [4] R. Chikkaraddy et al. Nature 535, 127 (2016).
- [5] X. Yan et al. arXiv 2309.08311 (2023).