MODELING 2D MATERIAL HETEROSTRUCTURES FOR OPTOELECTRONIC APPLICATIONS

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Scientific progress does not stand still, with it the requirements for the rapid operation of modern technologies are growing. Current materials' characteristics are not satisfying the growing standards for future development. Recently, materials such as graphene, MoS_2, and graphene oxide, which represent a group of 2D materials, have become more prominent to scientists. These materials have proven themselves as highly effective for wide applications in the fields of electronics and optoelectronics not only due to their remarkable electrical and optical qualities, but also because of their mechanical features such as high strength. The use of these materials opens up a completely new format for the vision of the current world of electronic devices. A good example of 2D materials is gallium selenide (GaSe). However, there remains a large set of physical and chemical properties that can be simultaneously exploited in this kind of materials for high-performance applications. This contribution provides computational and experimental results on the enhanced photonic properties of GaSe for applications in optoelectronics.

The objective of this work is to determine the light trapping capabilities of 2D semiconductor layers. We aim at providing a framework for engineering the physical dimensions of 2D layers to maximize the quantum efficiency and performance of optoelectronic devices. Thin layers of GaSe are investigated by the finite element method programming environment, which allows us to study the influence of light on the material using electromagnetic wave frequency domain physics. The Figure 1 illustrates the model of studying material – GaSe as a layer of 140 nm thickness placed on a highly ordered pyrolithic graphite (HOPG) substrate, illuminated by plane wave with λ=600 nm. The choice of the direction of the propagation vector is conditioned by the heterogeneous layered structure of GaSe. We perform a multiparametric sweep investigation as a function of GaSe thickness and incident wavelength that allows to maximize the light trapping efficiency of GaSe.

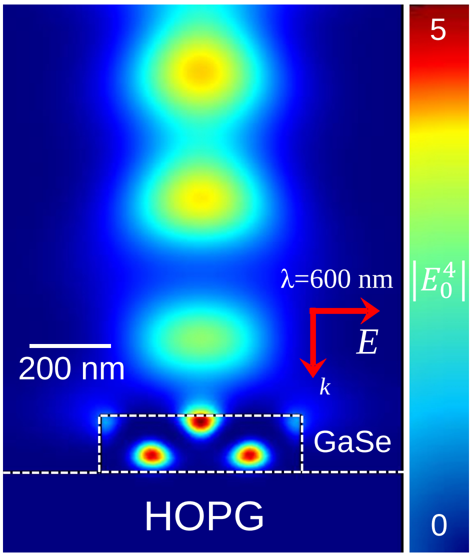

Figure 1: Finite element method simulation result of a GaSe layer on HOPG illuminated by a plane wave of 600 nm wavelength. The electric field enhancement reaches values of about 500% increase with respect to the magnitude of the incident excitation light.

We compare the simulation results with the experimental observations of electric field enhancement obtained by hyperspectral Raman spectroscopy imaging. As a Raman active probe, a 2 nm ultrathin layer of cobalt phthalocyanine (CoPc) was deposited on the GaSe/HOPG sample under ultra high vacuum conditions using organic molecular beam epitaxy. The hotspots, regions with highest electric field enhancement visible in Figure 1 are located at the top and bottom of the GaSe layer enhancing both the substrate and the CoPc layer on top of it. The computational result is in agreement with the experimental observations shown in Figure 2, where the Rayleigh and Raman signal from the substrate and CoPc are enhanced. This is exactly the effect that we hyphotesized. Our research results show that the light trapping capabilities of these layers used in optoelectronic devices could be largely increased.

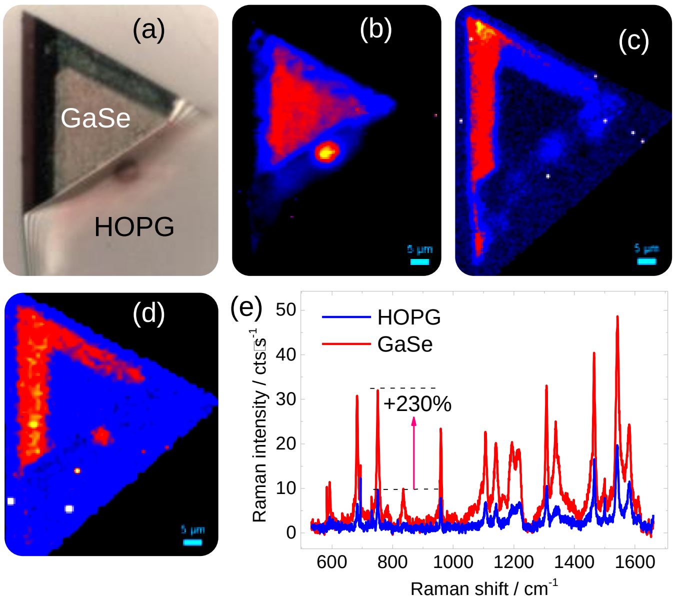

Figure 2: a) Optical microscopy image of a GaSe flake on HOPG. b) Rayleigh scattering image, c) CoPc Raman intensity for the mode around 1435 cm^{-1}, d) Raman signal from the G mode of HOPG, e) Raman spectra comparison for regions with and without GaSe.