Tuning the dimensionality of van der Waals materials for theranostic applications

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Two-dimensional (2D) layered transition metal dichalcogenides (TMDCs) have attracted tremendous research interests due to their unique properties for developing new-generation electronic and optoelectronic devices [1]. Nanostructures made from transition metal dichalcogenides represent unique platform for nanophotonics due to its high dielectric constants and nontrivial excitonic physics. The important feature of TMDCs nanoparticles (NPs) that distinguishes them from pure all-dielectric silicon NPs is the possibility of realization of Mie-exciton coupling regime that boosts light-matter interaction at the nanoscale manifesting itself in resonant enhancement of second harmonics generation [2], light scattering [3] and photothermal response [4]. However, it is worth noting that despite the recent significant progress in the field of dichalcogenide nanophotonics, the problem of nanostructuring of TMDCs remains open. On the one hand, it can be solved using standard technological approaches (such as lithography, ion beam etching). However, these methods have several limitations. For instance, they do not facilitate the production of spherical TMDCs nanoparticles. Meanwhile, various theranostic approaches rely on resonant spherical nanoparticles (NPs). These NPs enable both the visualization of nanoparticles within biological tissues and the treatment of malignancies through nanoparticle-enhanced phototherapy.

In this work we demonstrate nearly spherical nanoparticles of molybdenum and tungsten disulfides, diselenides and ditellurides (MoS₂, WS₂, MoSe₂, WSe₂, MoTe₂ and WTe₂) produced by femtosecond pulsed laser ablation of bulk target or nanoflake powder in deionized water. Structural and optical investigations have shown that that for all the NPs its structure is formed by polycrystalline inner part covered by fullerene-like outer shell. As a result, the preserved layered crystalline structure of laser ablated NPs combined with its variable size in the range 5-150 nm ensure the Mie-excitonic behaviour of its optical response. Such nanoparticles demonstrate exciting optical and electronic properties inherited from the TMDC crystals, due to preserved crystalline structure, which offers a unique combination of pronounced excitonic response and high refractive index value, making possible a strong concentration of electromagnetic field in nanoparticles. Moreover, it was found that the additional step of laser fragmentation of colloidal TMDCs NPs leads to appearance of amorphous fraction in the composition of produced nanoparticles and to an increased role of oxidation process during the growth of nanoparticles. Such partially oxidized MoSxOy nanoparticles provide efficient absorption of near-infrared radiation making them perfect candidates for biomedical theranostics applications.

References

- [1] Wang Q.H. et al., Nat. Nanotechnol., vol. 7, no. 11 (2012) 699
- [2] Popkova A.A. et al., Laser Photonics Rev. 16, (2022) 2100604
- [3] Tselikov G.I. et. al., Proc. Natl. Acad. Sci. U. S. A., vol. 119, no. 39 (2022) e2208830119
- [4] Chernikov A.S. et. al., J. Mater. Chem. C, 11 (2023) 3493