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Recent Trends in SERS: Sensing and DFT Application

Guest Editor:

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Message from the Guest Editor

Surface-enhanced Raman spectroscopy (SERS) has proven to be an invaluable technique for the detection and identification of organic substances, even in trace levels. This technique is based on the large local enhancement of the incident electromagnetic field in the proximity of the metal nanoparticles, as a consequence of localized surface plasmon resonance. This resonance gives rise to large enhancements of the cross-section for optical spectroscopy, such as SERS. Thus, this technique can be successfully used for the study of very insoluble compounds in water, as very low concentrations are detected, even in trace levels. Its ultrahigh sensitivity, tougher with high selectivity, makes the SERS technique extremely appropriate for sensing applications in many different fields. The aim of this Special Issue is to provide an overview of the latest research in the field of the application of DFT calculation methods for the study of several aspects related to SERS spectroscopy, such as the type of molecular adsorbance on the SERS substrates, the existence of a charge transfer mechanism in the metal-molecule system and vibrational analysis of the adsorbate.

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Message from the Editor-in-Chief

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