PHYSICAL AND TECHNOLOGICAL SCIENCES

Molecular Vibrational Spectroscopy

Vilnius University

Keywords: *FTIR spectroscopy; Raman spectroscopy; low frequency Raman; SERS; matrix isolation; cancer spectral markers; conformational analysis; thin films*

Research group activities

Modern vibrational spectroscopy is frequently used in many fields of science and industry for qualitative and quantitative analysis of solid, liquid and gaseous substances. Main limiting factors of wider application of the method are (I) limited sensitivity and (II) difficulties with analysis of polymeric and biological substances related to very complex structure of their spectra. These problems can be solved using some smart methods of sampling.

Since modern spectroscopic methods are very informative and featuring nondestructivity, potential for express analysis, reasonable price, they are in great demand for various scientific, diagnostic solutions.

For many years our research team is focused on:

- Qualitative and quantitative spectral analysis of gases, solids, solutions and composites;
- Raman and mid-infrared chemical imaging of surfaces and films;
- Conformational analysis of organic substances;
- Qualitative and quantitative spectral analysis of biological crystals and fluids;
- Spectroscopic diagnostics of cancer cells;
- Development of methods of SERS spectroscopy for various substances to approach the theoretical sensitivity limit. Intensity of Raman spectra (as well as sensitivity of the method) can be increased substantially by adsorbing molecules of interest at metal nanoparticles or at nanoscale corrugated metal surface. In such a way SERS spectra can be produced offering sensitivity of qualitative and quantitative analysis up to 10-6 M.

Proposal

The group offers services related to the research activities of the group.

We are searching for partners in the frame of HORIZON 2020 to apply our methods of Raman and infrared spectroscopy in various fields of photonics, semiconductors and nanoscience.

Designing of FTIR express analyser of cancerous biological tissue, based on fiber ATR-probe, which can act as smart surgical knife.

Meet our team

Our group consists from 7 members, including experienced and young scientists. Average age of the group is 33 years.

Leader of the group - Prof. Dr. **Valdas Šablinskas**

Researchers - Assoc. Prof. Dr. **Justinas Čeponkus** and Assoc. Prof. Dr. **Vidita Urbonienė**

PhD students - **Martynas Velička**, **Rasa Platakytė**, **Sandra Tamošaitytė** and **Joana Stocka**

Research outcomes

Recent publications

- **V. Vajda, M. Pucetaite, S. McLoughlin, A Engdahl, J. Heimdahl, P. Uvdal**, Molecular signatures of fossil leaves provide unexpected new evidence for extinct plant relationships, Nature Ecology and Evolution, doi:10.1038/s41559-017-0224-5 (2017).
- **M. Pucetaite, S. Tamosaityte, R. Galli, V. Sablinskas, G. Steiner,** Microstructure of urinary stones as studied by means of multimodal nonlinear optical imaging, Journal of Raman Spectrocopy, (online Early View, DOI: 10.1002/jrs.4985) (2016).
- **G. Steiner, G. Preusse, C. Zimmerer, M. Krautwald-Junghanns, V. Sablinskas, H. Fuhrmann, E. Koch, T. Bartels,** Label free molecular sexing of monomorphic birds using infrared spectroscopic imaging, Talanta, 150,155–161 (2016).
- **M. Pucetaite, M. Velicka, J. Pilipavicius, A. Beganskiene, J. Ceponkus, V. Sablinskas,** Uric acid detection by means of SERS spectroscopy on dried Ag colloidal drops. Journal of Raman Spectrocopy, vol. 47(6), p. 681-686 (2016).
- **J. Ceponkus, M. Jonusas, C. P. Cotter, M. Pucetaite, V. Aleksa, G. A. Guirgis and V. Sablinskas,** Structural studies of 1,1-dimethyl-2-oxy-1-silacyclohexane by means of matrix isolation infrared absorption spectroscopy, The Journal of Physical Chemistry A, 119 (11), 2721–2726 (2015).

Currently the group is involved in 4 years project financed by Lithuanian science council in the frame of National program “Healthy aging”.

We regularly provide spectroscopic services for some high-tech companies, such as SPRANA, ALTECHNA, OPTOLITA and other companies.

Resources

Our research group is equipped with a set of modern spectral instruments, which allow using interaction of light with matter for analysis of substances in wide spectral range from 200 nm to 1 mm.

Contacts

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