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AnalytiX

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BIT's 7th Annual Conference of

AnalytiX-2019

Theme: Exploring Innovative Advances and Applications

Conference Handbook

Title: Advances in FTIR Spectroscopy of Surface Species

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Abstract

Vibrational spectroscopy is the most powerful non-destructive method for surface studies. Spectra of surface functional groups and adsorbed test molecules provide information on the nature of active sites, their strength and concentration. At low-temperatures it is possible to see the spectra of CO, NO, H_2 N_2, CHF_3 or other simple molecules that do not adsorb at room temperature and characterize surface OH-groups, electron-accepting or electron-donating sites. Variable temperature spectroscopy enables us to study thermodynamics of surface processes and get information about the mechanism of catalytic reactions. To trap unstable intermediates of catalytic processes we can follow spectra evolution with temperature and their structure can be clarified using the isotopic substitution.

Some adsorption products cannot be stabilized at low temperatures, but arise at the surface as a result of thermal excitation. So, besides the usual C-bonded structure CO forms with the cations in zeolites energetically less favorable O-bonded species. Such linkage isomerism was established for some other adsorbed species, such as cyanide ion CN^- produced by HCN dissociation.

FTIR spectra are sensitive to lateral interactions between the adsorbed species, which shift the bands of test molecules or complicate their contours. Co-adsorption of acidic and basic molecules leads to mutual enhancement of adsorption. Acidity of surface sites can be increased by adsorbed acidic molecules, this explains the superacidity of oxides doped with SO_4^{2-}. By means of isotopic dilution this static interaction can be distinguished from the dynamic one. The latter, or resonance dipole-dipole interaction, accounts for the vibrational energy exchange in the adsorbed layer. Its spectral manifestation provides additional information on the geometry of surfaces.

Quantitative spectral analysis of surface sites is not possible without the knowledge of absorption coefficients of test molecules. Quantum chemical calculations and electrostatic approach predict the correlation between the frequency shifts on adsorption and the absorption coefficients, in a fair agreement with the experimental data.

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Biography

Alexey Tsyganenko, Professor of Physical Faculty of St. Petersburg State University, Head of a Chair. Graduated in 1971, Ph.D. 1975. Since 1983 Head of the research group of Infrared Spectroscopy, V. A. Fock Institute of Physics of the University. Participated in scientific researches in France, Germany, the Netherlands, Spain and Finland. The list of publications includes over 125 papers, 2500 citations.