

CATALYSIS AND LOCALIZED ANHARMONIC VIBRATIONS

Conference by Dr. **Vladimir Dubinko**, from
Kharkov Institute for Physics and Technology,
Ukraine

Premises: **Seminario del Departamento de Física
Aplicada 1, ETSI Informática, Avda Reina
Mercedes s/n; 41012-Sevilla** (Planta baja: G0.81)
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13:00 to 13:45.**

Conference organized by the **JFR Archilla** and the
Group of Nonlinear Physics of the University of Sevilla



Abstract: A new mechanism of catalysis is discussed, which is based on the rate-promoting effect of large-amplitude localized anharmonic vibrations (LAV), which can excite atoms at specific ‘active sites’ rather strongly, giving them energy far exceeding the energy of thermal vibrations for hundreds of oscillation periods. Localized anharmonic vibrations induce modulation of the activation energies (free energy barriers between reactants and products) resulting in a drastic amplification of the reaction rates, which can be described by a simple analytical expression in the adiabatic limit. The striking site selectiveness of anharmonic excitation dynamics in the presence of spatial (quenched) disorder makes these nonlinear vibrations viable candidates to play the role of ‘active modes’ in the catalytic process in various physical, chemical and biological systems.

