Chemical and Nuclear Catalysis Mediated by the Energy Localization in Hydrogenated Crystals and Quasicrystals

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Catalysis is at the heart of almost every chemical or nuclear transformation process, and a detailed understanding of the active species and their related reaction mechanism is of great interest. An important parameter of the reaction kinetics is the *activation energy*, i.e. the energy required to overcome the reaction barrier. The lower is the activation energy, the faster the reaction rate, and so a catalyst may be thought to reduce somehow the activation energy. Dubinko et al [1] have shown that in a crystalline matrix, the activation energy may be reduced due to *localized anharmonic vibrations* (LAVs) of atoms, LAV can be excited thermally or by irradiation, resulting in a drastic acceleration of *chemical reaction* rates driven by thermally-activated 'jumps' over the reaction barrier due to the time-periodic modulation of the barrier height in the LAV vicinity.

At sufficiently low temperatures, the reaction rate is controlled *by quantum zero-point vibrations (ZPV)* rather than by thermal fluctuations. Large amplitude atomic motion in LAVs may result in time-periodic driving of adjacent potential wells occupied by hydrogen ions (protons or deuterons) upon hydrogenation. This driving is shown to result in the increase of amplitude and energy of zero-point vibrations (ZPVs). Based on that, we demonstrate a drastic increase of the D-D or D-H fusion rate with increasing number of modulation periods evaluated in the framework of Schwinger model [2], which takes into account suppression of the Coulomb barrier due to ZPVs, which is further enhanced by LAVs. In this context, we will present numerical solution of Schrodinger equation for a particle in a non-stationary double well potential, which is driven time-periodically imitating the action of a LAV [3]. We show that the rate of tunnelling of the particle through the potential barrier separating the wells can be enhanced enormously by the driving in a certain frequency range.

We will present atomistic simulations of LAVs in the crystal lattice of Ni, Pd, Ti-Zr-Ni and in their quasicrystaline nanoclusters.

We will present experimental results on the interaction of the Ni, Pd and Ti-Zr-Ni crystals and quasicrystals with hydrogen and deuterium under thermal equilibrium and under gamma irradiation, which is introduced as an efficient tool for the athermal production of LAVs.

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