# Energy Localization in Hydrogenated Metals: Applications to the Rate Theory

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**Abstract:** Energy localization in crystals manifest itself as *intrinsic localized modes* or *discrete breathers* (DBs). We present atomistic simulations of DBs in nickel, palladium and their hydrides. Large amplitude atomic motion in DBs may result in time-periodic driving of adjacent potential wells occupied by hydrogen ions (protons or deuterons). This driving has been shown to result in the increase of amplitude and energy of zero-point vibrations and in broadening of the wave packet. In this context, we 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 DB. We show that the rate of tunneling of the particle through the potential barrier separating the wells is drastically enhanced by the driving with a resonant frequency ranging from w0 to 2w0, where w0 is the eigenfrequency of the potential well. The effect increases strongly with increasing amplitude of the driving. These results support the concept of DB mediated catalysis and extend it to low temperatures where quantum tunneling prevails over thermal activation controlling the reaction rates in solids.
**Keywords:** Discrete breathers, Quantum Tunneling, Rate Theory, Catalysis.