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Discovery of Dynamics of Jahn-Teller Effect DAN LIU — Taking S=1/2 $NaSiTi_2O_6$ as example, we discovered the dynamics of the Jahn-Teller effect of solids by extending the molecular frontier orbital theory from chemistry to solid state physics. At the orbital and spin levels, the dynamics of the Jahn-Teller effect is exposed to involve spin flipping and spontaneous orbital transition that is driven by the spin-orbital coupling to keep the angle momentum reservation. The orbital transition leads to a dramatic structural change, i.e., the JT distortion. In analogue to the singlet-triplet intersystem crossing of photochemistry, the JT effect is a non-adiabatic process, associated with the first-order phase transition. The JT effect agrees well with the low-dimensional, S=1 Haldane gap on the basis of the antimagnetic Heisenberg model, if emphasizing that the S=1 parameter of Haldane gap indicates the parallel spins of neighboring orbitals, rather than the on-site parallel spins. We provide insight to understanding of the unusual structural, magnetic properties of S=1/2 $NaTiSi_2O_6$, as well as the S=1$LiVGe_2O_6$ and S=3/2 $LiCrGe_2O_6$.

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