THEORETICAL STUDY OF THE METHANE STRETCHING VIBRATIONAL ENERGY LEVEL STRUCTURE CLOSE TO A NICKEL SURFACE

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A vibrational Hamiltonian has been constracted for methane to study stretching vibrational energy level structure when the molecule approaches a nickel surface. A local mode Hamiltonian is used for an isolated molecule. A LEPS potential energy function is chosen to describe surface-molecule interactions. Stretching vibrational energy levels have been calculated variationally at different molecular distances and orientations from the surface. In the case of the local mode pairs of states ($1000A_1/F_2$) and ($2000A_1/F_2$), the symmetric A_1 states decrease in energy and the antisymmetric F_2 states stay almost constant in energy and become stretching states of CH_3 as the methane molecule approaches the surface. This indicates that the excitation of the symmetric states would have an effect on the chemical reactivity close to the surface but the excitation of the antisymmetric states would not.