[P7] The effect of molecular vibrations on the binding of a positron to polyatomic molecules

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The positron, which is the anti-particle of the electron, is now widely used in both scientific and technological areas such as physics, chemistry, material science, medicine, and their interdisciplinary areas. Positrons injected into a liquid or solid induce various processes such as an ionization or electronic excitation of atoms/molecules, the formation of a metastable bound state of a positron and an electron, formation of positron-molecular complexes, etc., before the positron undergoes a pair-annihilation with an electron. The detail mechanism of such processes, however, are still unclear in the molecular level.

A positron affinity (PA), which is a binding energy of a positron to an atom or molecule, is one of the most important properties for studying positron attachment process. The PA values have now been experimentally measured by Surko and co-workers for many molecular species such as some hydrocarbons (alkanes, alkenes, and aromatics), alcohols, and halogenated hydrocarbons [1-3]. Their PA measurement is based on the vibrational Feshbach resonance (VFR) by incident low-energy positrons, in which the formation of a positron-molecular complex at the molecular vibrational excited states is suggested. Thus, in order to elucidate the mechanism of the positron binding to molecules in vibrational excited states in detail, the theoretical analysis including the effect of the molecular vibrations is quite indispensable. In most theoretical analyses of positron-molecular complexes reported so far, however, the positron binding to molecules as well as the PA value has been analyzed only at the molecular equilibrium geometry.

In this study, thus, we developed a new theoretical method for analyzing the effect of molecular vibrations on positron affinities in order to elucidate the mechanism of the positron binding to molecules in vibrational excited states. The method is based on both the anharmonic vibrational state theory using quantum Monte Carlo (QMC) technique [4] and ab inito multi-component molecular orbital (MC_MO) theory [5,6] that enable us to analyze an electronic and positronic wave function. To demonstrate the effect of molecular vibrations to the positron bindings with our method, we analyzed the characteristic features of the positron binding to some small molecules such as hydrogen cyanide (HCN), formaldehyde (CH2O) molecules, etc. The detail of theoretical method and results will be presented on the day.

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