Journal of Physics: Conference Series **635** (2015) 072085 doi:10.1088/1742-6596/635/7/072085

Theoretical analysis of positron-attachment to small molecules: Vibrational enhancement of positron affinities

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Synopsis To theoretically demonstrate the binding of a positron to small polarized molecules, we have calculated the vibrational averaged positron affinity (PA) values for small molecules with multi-component quantum Monte Carlo and molecular orbital methods. Our most accurate prediction of the vibrational averaged PA values at the fundamental and overtone states for formaldehyde molecule are 31 and 36 meV, respectively.

The positron is now widely used in both scientific and technological areas. The detail mechanism of such processes, however, is still unclear in the molecular level. A positron affinity (PA) value, which is a binding energy of a positron to an atom or molecule, has now been experimentally measured by Surko and co-workers for many molecular species [1], based on the vibrational Feshbach resonance by incident low-energy positrons. Thus, in order to elucidate the mechanism of the positron binding to molecules, the theoretical analysis including the effect of molecular vibrations is indispensable.

In this study, we developed a new theoretical method for analyzing the effect of molecular vibrations on positron affinities. Our strategy is based on ab initio multi-component quantum Monte Carlo (QMC) [2] and molecular orbital (MCMO) [3, 4] methods for the electronic and positronic wave functions simultaneously, and the anharmonic vibrational state theory using quantum Monte Carlo (QMC) method [5, 6]. In the case of formaldehyde (CH_2O) molecule, the vertical PA value at the equilibrium position is predicted as +25(3) meV with QMC calculation. Applying the anharmonic vibrational analysis, the vibrational excitation of the C=O stretching mode drastically enhances the PA value, whereas the excitation of CH_2 rocking mode deenhances it. We confirmed that such PA variations arise from the change in both permanent dipole moment and dipole-polarizability at each vibrational excited state. Our most accurate prediction of the vibrational averaged PA values at the fundamental and overtone states are 31 and 36 meV, respectively, which strongly supports the conclusion that a positron can bind to formaldehyde [6].

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