

In Vivo Machine Learning in Synthetic Biology

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Description

First-principles methods for time-resolved angular resolved photoelectron spectroscopy play a pivotal role in providing interpretation and microscopic understanding of the complex experimental data and in exploring novel observables or observation conditions that may be achieved in future experiments. Here we describe an efficient, reliable and scalable first-principles method for tr-ARPES based on time-dependent density functional theory including propagation and surface effects usually discarded in the widely used many-body techniques based on computing the non-equilibrium spectral function and discuss its application to a variety of pump-probe conditions. We identify four conditions, depending on the length of the probe relative to the excitation in the materials on the one hand and on the overlap between pump and probe on the other hand. Within this paradigm different examples of observables of time-resolved ARPES are discussed in view of the newly developed and highly accurate time-resolved experimental spectroscopies.

Classical Covalent-Bond

According to the classical covalent-bond (CVB) model, the two s and two p valence electrons in C, Si, and Ge crystals with diamond structure adopt an equivalent sp³ structure and form four covalent bonds between an atom and its four adjacent atoms. Therefore, the four valence electrons (sp³) per atom should have the same energy state. However, many experimental results indicate that the valence electrons of these element crystals have different binding energies. Therefore, in this paper, we propose a local valence electron (LVE) model for these materials, on the basis of valence electron spectra for the C, Si, and Ge crystals: The states of the four valence electrons per atom in these crystals are similar to those in the free atoms (s²p²), except that the shape of their outer electron cloud shells deviates from the ball shell distribution in the crystals, forming positive ions and equivalent-negative-electrical-charge centers. One of the important reasons why all the valence electrons of diamond are local electrons is that free C atom has high first ionization energy, 11.26 eV, being much higher than those of all the metal atoms. This LVE model is accordance with that diamond has wide energy gap (5.4 eV) in the energy band theory, which forbids electron transition

from the filled valence band to the vacant conduction band. In this work, a computational study on electron interactions with diazene (N₂H₂) and hydrazine (N₂H₄) was performed; two conformations of N₂H₂ (–N₂H₂ and –N₂H₂) were considered. Differential cross sections (DCS), integral cross sections (ICS), and momentum transfer cross sections (MTCS) for elastic scattering as well as total cross sections (TCS) and total absorption cross sections (TACS) were explored at incident energies from 0.1 to 500 eV. A molecular complex optical potential approach combined with Padé approximants was used for describing the electron–molecule collision dynamics and solving the scattering equations. Marked differences were noticed when the DCS for elastic electron–N₂H₂ scattering were compared to the corresponding results for electron–N₂H₂ (particularly at low incident energies and small angles), a behavior which was assigned to the existence of a permanent dipole moment in the case of the –N₂H₂ molecule; results regarding N₂H₄ were found to be considerably more similar to those determined for –N₂H₂. In terms of ICS and MTCS, results obtained for –N₂H₂ presented a first peak at 1.15 eV (originating from the continuum symmetry and being related to the resonance arising from the nitrogen-nitrogen bond) and another at around 10 eV. These peaks can be related to the moiety and to the existence of the bonds, respectively. Interestingly, no peaks were clearly observed in –N₂H₂ ICS and MTCS while only the peak at around 10 eV was (barely) seen in the MTCS of N₂H₄, even without employing the Born-closure procedure. Hence, conformation plays a major role in probing the resonances for the N₂H₂ molecule, being the strong dipole moments responsible for masking the structures in the case of –N₂H₂ (as well as eventual additional peaks in N₂H₄). TACS results were found to be (practically) the same for both conformations of N₂H₂ at the energy range probed, being systematically lower than N₂H₄ TACS. In addition, the maxima of absorption was found at 70 eV for N₂H₄, which is slightly shifted when compared to the maxima probed for –N₂H₂ and –N₂H₂ (observed at 80 eV).

Micro Channel Plate Detector

A micro channel plate detector with a large open area ratio (nominally 90%) has been installed in a magnetic bottle electron spectrometer in order to improve the coincidence efficiency in multi-electron–ion coincidence measurements. The overall detection efficiency of the magnetic bottle

spectrometer is determined to be ~70% for electrons with kinetic energies of up to at least 530 eV and ~85% for XeZ^+ ($Z > 3$) ions. The usefulness of the improved detection efficiency in multi-electron-ion coincidence spectroscopy is demonstrated by a six-fold coincidence measurement about the quadruple Auger decay of the Xe $3d_{5/2}$ core-hole state. We present the photodetachment microscopy of the singly charged negative ions using the double pulse with a frequency near the ionization threshold in the presence of the time-dependent external electric field. In the presence of time-dependent electric field, the number of photoelectron trajectories contributing to the electron flux at a space-time point at the detector may be more than two. We demonstrate that the relative flight times of the classical trajectories, to reach a point at the detector plane can be calculated by observing the photoelectron flux at a particular time at the detector and scanning the second pulse by varying the time delay between the two coherent laser pulses.

Moreover, investigating the photoelectron flux, we have found that the flux distribution can be controlled by the relative phase difference between the two coherent pulses separated by a short time delay, at spatial and temporal points where the classical trajectories associated with photoelectron emerging at different pulses arrive at the detector simultaneously and exhibit interference. The temporal and spatial photoelectron flux distribution oscillates as a function of the relative phase difference between the pulses. The time-dependent quantum propagator approach with stationary phase approximation is linked analytically with the time-dependent closed orbit theory.