

# Stability of Auger final dicationic states of core-ionized N<sub>2</sub> molecules studied by Auger-electron ion coincidence measurements

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**Synopsis** We present experimental results for AEPICO measurements following core photoionization of N<sub>2</sub> molecules, with using an AEPICO spectrometer in which a toroidal electron energy analyzer and an ion momentum spectrometer are installed.

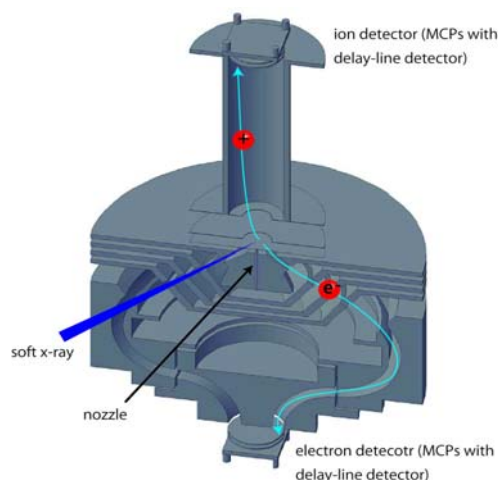
Absorption of a soft x-ray creates a core hole in a molecules. A core hole state is unstable and usually leads to Auger decay for light elements. This Auger decay process produces various valence-hole configuration. Although the dicationic states are generally unstable and come apart into ionic fragments, quasi-bound or metastable dicationic states are known to exist. In this work, we investigate a stability of Auger final states of core ionized N<sub>2</sub> molecules with Auger-electron ion coincidence measurements.

The Auger-electron-ion coincidence measurements for core ionized N<sub>2</sub> molecules were carried out on the undulator beamline BL6U at UVSOR. The radiation from an undulator was monochromatized by a variable included angle varied line-spacing plane grazing monochromator. The electrons ejected at 54.7° with respect to the electric vector of the ionization light were analyzed in energy by double toroidal analyzer (DTA), while ions were extracted from the interaction region into the momentum spectrometer by a pulsed electric field according to the electron detection. Arrival positions on the detector and time-of-flights of ions were recorded for every event. The pass energy of the DTA was set to 200 eV for observing resonant Auger electrons. The energy resolution was about 1.2 eV. All signals from electron and ion detectors were recorded with an 8ch TDC board. We used photon energies of 450 eV. Here we note that ion time-of-flight can't be used to distinguish two ion species of N<sub>2</sub><sup>2+</sup> and N<sup>+</sup> due to the same mass-to-charge ratio. Since fragmentation process give large kinetic energy, we can identify ion species with their kinetic energies of ions.

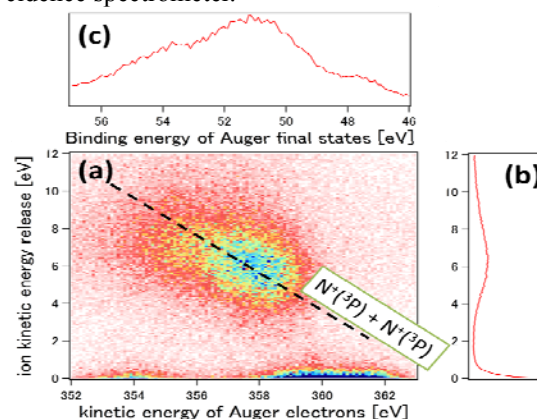
Figure 2 (a) shows an Auger-electron ion coincidence map for core-ionized N<sub>2</sub> molecules. The vertical and horizon axes of the map correspond to the kinetic energy of ion and Auger electron, respectively. Figure 2(b) and (c) shows total ion kinetic distributions and Auger electron spectrum with a binding energy scale. As shown in Fig. 2(b), ion kinetic energy distribution has two peaks at 0 eV and 6 eV. This represents that ions with nearly zero kinetic energy are N<sub>2</sub><sup>2+</sup> while energetic ions are N<sup>+</sup> fragment ions.

For (N<sup>+</sup>, N<sup>+</sup>) fragmentation process, we found that strong correlation between Auger-electron and ion kinetic energies, as shown in Fig.2(a). The slope of -1 means that these fragmentations reach a same fragmentation limit. From NIST Atomic Database, we found that they correspond to N<sup>+</sup>(3P) + N<sup>+</sup>(3P) fragmentations.

Auger final states ranging from 50 to 54 eV in binding energy scale are unstable and immediately lead to fragmentations. From the theoretical works[1], these Auger final states mainly comes from the 1Δg(1πu-2) configuration. Conversely Auger final states ranging from 46 to 50 eV and from 54 to 56 eV are stable. These Auger final states mainly comes from 3σg-2 and 2σg-11πu-1 configurations. In conclusion, we found that two 1πu bonds of N<sub>2</sub> molecules play an important role on a stability of dicationic states.



**Figure 1.** A schematic view of Auger electron-ion coincidence spectrometer.



**Figure 2.** (a) Auger-electron ion coincidence map for core-ionized N<sub>2</sub> molecules. The spectra (b) and (c) shown at the right and top panels represents the total ion kinetic distribution and Auger electron spectra in binding energy scale, respectively.

[1] H. Agren, J. Chem. Phys. **75** (1982) 1267

