Abstract Submitted
for the DAMOP13 Meeting of
The American Physical Society

The Cooper-like minimum in the HHG of N_2: A TDDFT study[1]

XI CHU, The University of Montana, GERRIT GROENENBOOM, Radbboud University Nijmegen — A minimum at ∼39 eV is observed in the high-harmonic-generation spectra of N2 for several laser intensities and frequencies. This minimum appears to be invariant for different molecular orientations. We reproduce this minimum for a set of laser parameters and orientations in time-dependent density-functional-theory calculations, which also render orientation-dependent maxima at 23-26 eV. Photon energies of these maxima overlap with ionization potentials of excited states observed in photoelectron spectra. Time profile analysis shows that these maxima are caused by resonance-enhanced multiphoton excitation. We propose a four-step mechanism, in which an additional excitation step is added to the well-accepted three-step model. Excitation to a linear combination of Rydberg states c_4? $^1\Sigma_u^+$ and c_3 $^1\Pi_u$ gives rise to an orientation-invariant minimum analogous to the "Cooper minimum" in argon. When the molecular axis is parallel to the polarization direction of the field, a radial node goes through the atomic centers, and hence the Cooper-like minimum coincides with the minimum predicted by a modified two-center interference model that considers the de-excitation of the ion and symmetry of the Rydberg orbital.

[1]This work is supported by NSF Award No. PHY-0855676.

Xi Chu
The University of Montana

Date submitted: 04 Apr 2013 Electronic form version 1.4