CFEL SCIENCE

SEMINAR

26th April 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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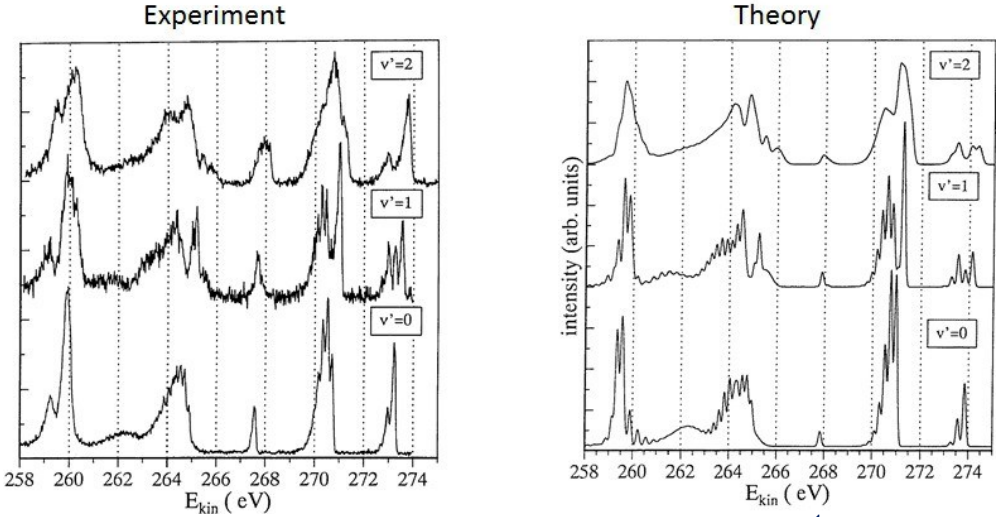
The one center approximation for molecular Auger transition rates

The one-center approximation, a simple method for the calculation of molecular Auger electron spectra, is shown to (a) provide accurate predictions for molecular Auger electron spectra of 1*s*, 2*p* and, 3*d* core-hole species; (b) reproduce the angular distribution and spin-polarisation of Auger electrons; (c) be applicable to small molecules as well as to larger ones as well as to clusters, surfaces or to aggregates; (d) give rise to a set of "thumb rules" which allow to relate the Auger decay to electronic structure properties. The concept of the one center approximation is sketched. Theoretical *KVV* Auger electron spectra of even extended systems and vibrationally resolved spectra as well as of 2*p* hole states underline the applicability of the method. Auger transition rates of 3*d* ionised HBr are also well reproduced which is remarkable due to low kinetic energy of those Auger electrons. By introducing the scattering phases of the Auger continuum channel the angular distributions of Auger electrons can be determined in good agreement with experimental anisotropy parameters β as well as the angular distribution of fixed-in-space molecules.



Vibrationally resolved resonant Auger electron spectrum of C $1s^{-1}$ 2π excited CO.

Host: Robin Santra – CFEL-DESY Theory Division