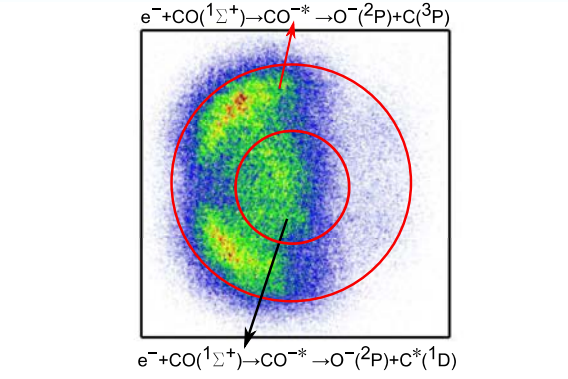
Dissociative Electron Attachment to CO molecule probed by velocity slice imaging technique



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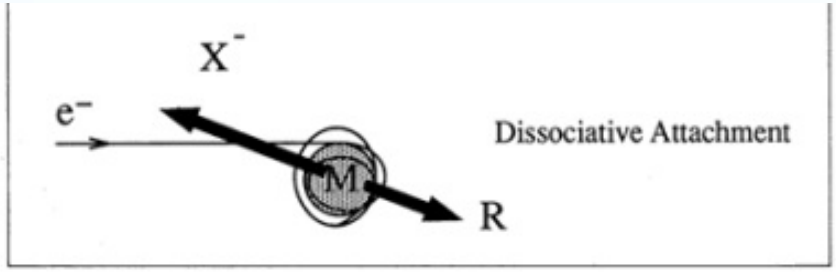
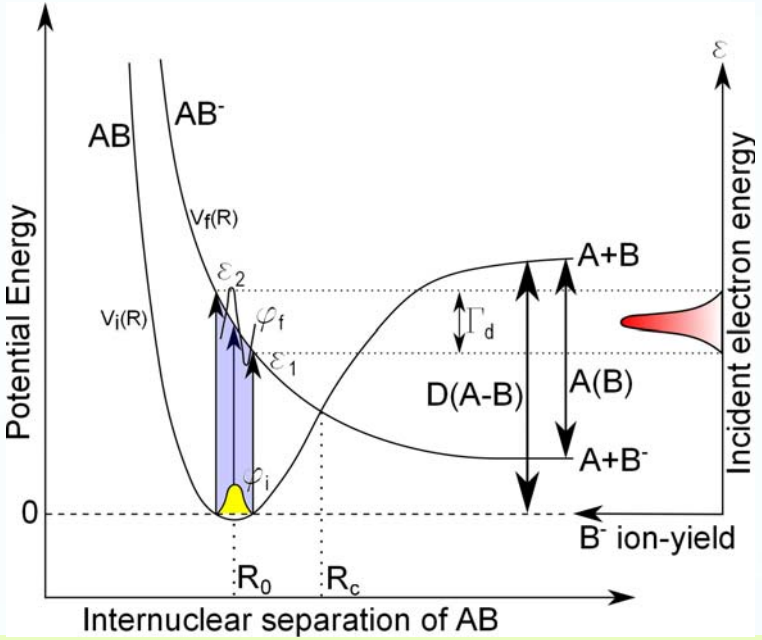
28th July, 2017





Cross Sections

Kinetic Energy

Angular Distribution

Importance

Applications and Dynamics

Dissociative Electron Attachment (DEA)

Step I : $AB + e^- \rightarrow AB^{-*}$ (Attachment)

Step II : $AB^{-*} \rightarrow AB^{*} + e^-$

(Auto-detachment)

or

$AB^{-*} \rightarrow A + B^-$

(Dissociation)

Dissociative Electron Attachment to CO

$$e^- + \mathrm{CO}(^1\Sigma^+) \rightarrow \mathrm{CO}^{-*} \rightarrow \mathrm{O}^-(^2P) + \mathrm{C}(^3P)$$ Process I

$$e^- + \mathrm{CO}(^1\Sigma^+) \rightarrow \mathrm{CO}^{-*} \rightarrow \mathrm{O}^-(^2P) + \mathrm{C}^*(^1D)$$ Process II

$$e^- + CO(^1\Sigma^+) \rightarrow CO^{-*} \rightarrow O^-(^2P) + C^*(^1S)$$ Process III

Threshold energy:

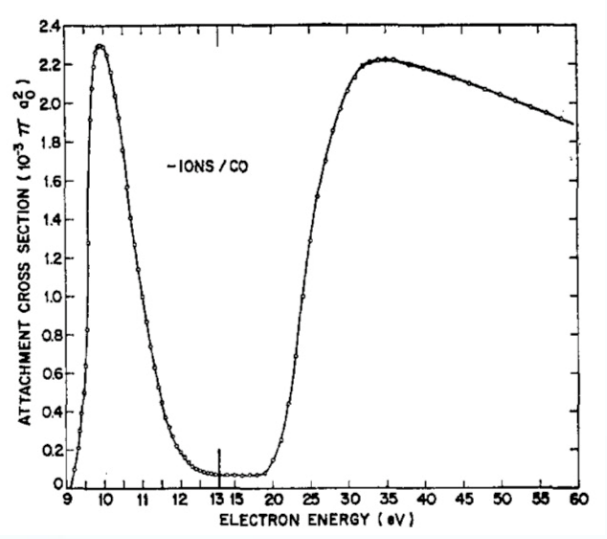
Process I: 9.62 eV

Process II: 10.88 eV

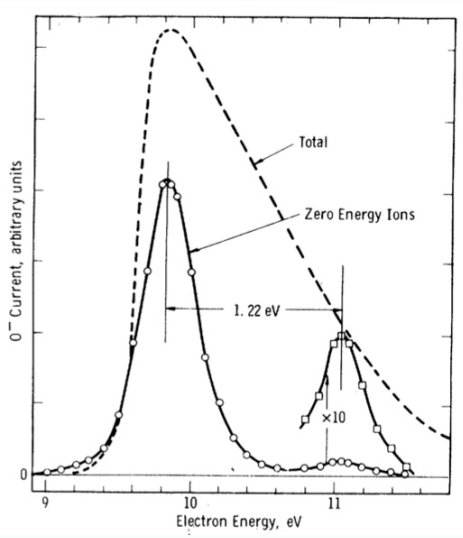
Process III: 12.30 eV

Thermochemical parameters

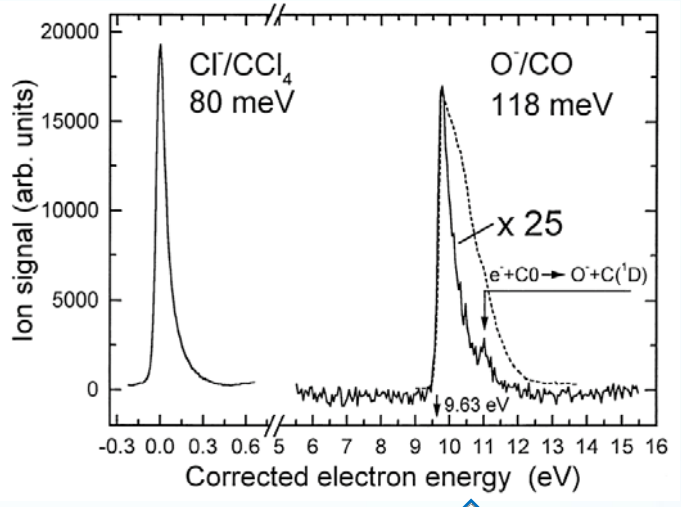
D(C-O) = 11.09 eV
EA(O) = 1.47 eV
C(^{3}P) = 0.0 eV
C*(^{1}D) = 1.26 eV
C*(^{1}S) = 1.42 eV



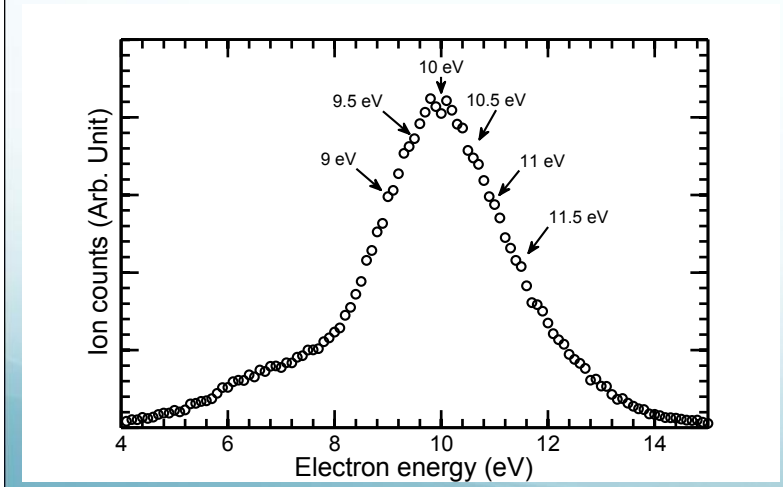
Rapp and Briglia, J. Chem. Phys. **43** (1965) 1480



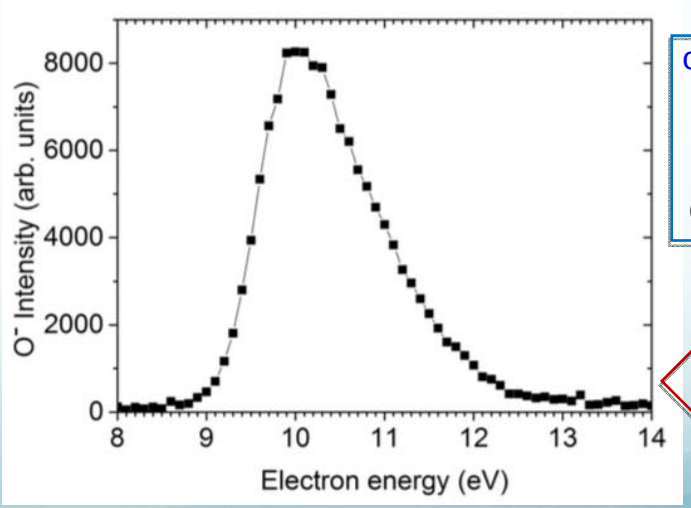
P. J. Chantry, Phys. Rev. **172** (1968) 125



G. Denifl et al., Chem. Phys. Lett., **288** (1998) 105



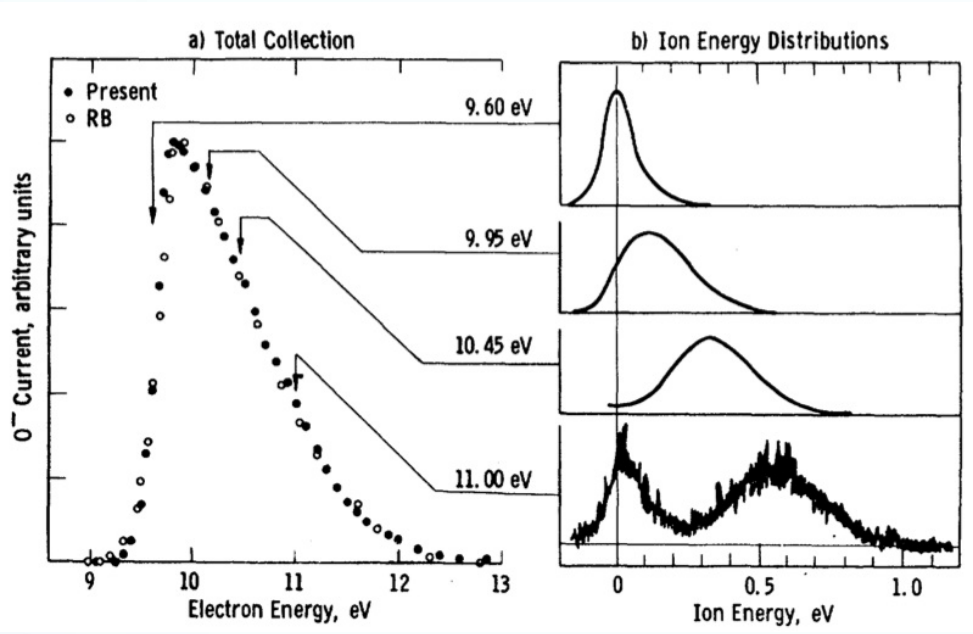
Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130

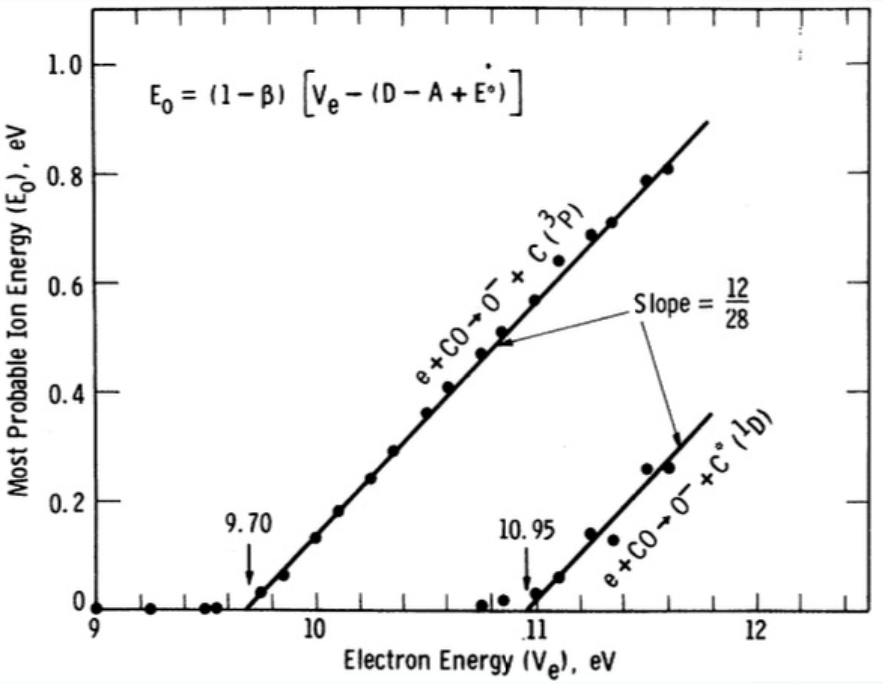


K. Gope et al., Eur. Phys. J. D. **70,** 134 (2016).

- Electron monochromator
- Quadupole mass filter
- Process II : ~ 5%

Imaging spectrometers





P. J. Chantry, Phys. Rev. **172** (1968) 125

Rapp and Briglia, J. Chem. Phys. **43** (1965) 1480

Process I: 9.62 eV

Process II: 10.88 eV

- Total collection: by Retarding Potential Difference
- Kinetic energy distribution using Wien filter
- **Separation between two peaks => excitation energy of $C^*(^1D)$ [Process II]**

Angular Dependence of Fragment Ions from DEA

*(O'Malley and Taylor; Phys. Rev., **176** (1968) 207)*

$$I(k,\theta,\phi) = \sum_{|\mu|} \Big| \sum_{l=|\mu|}^{\infty} a_{l\mu}(k) Y_{l\mu}(\theta,\phi) \Big|^2$$

*Azria et.al., J. Phys. B **12**, 679 (1979)*

$$f(\theta) \propto \frac{1}{2\pi} \int_0^{2\pi} \Big| \sum_{l,m,\varepsilon} i^l exp(i\delta_l) a_{lm}^{\varepsilon} X_{lm}^{\varepsilon *}(\theta,\phi) \Big|^2 d\phi$$

k : incident electron momentum; $a_{l\mu}$ (k) : energy dependent expansion coefficients; $Y_{l\mu}(\theta,\phi)$: spherical harmonics

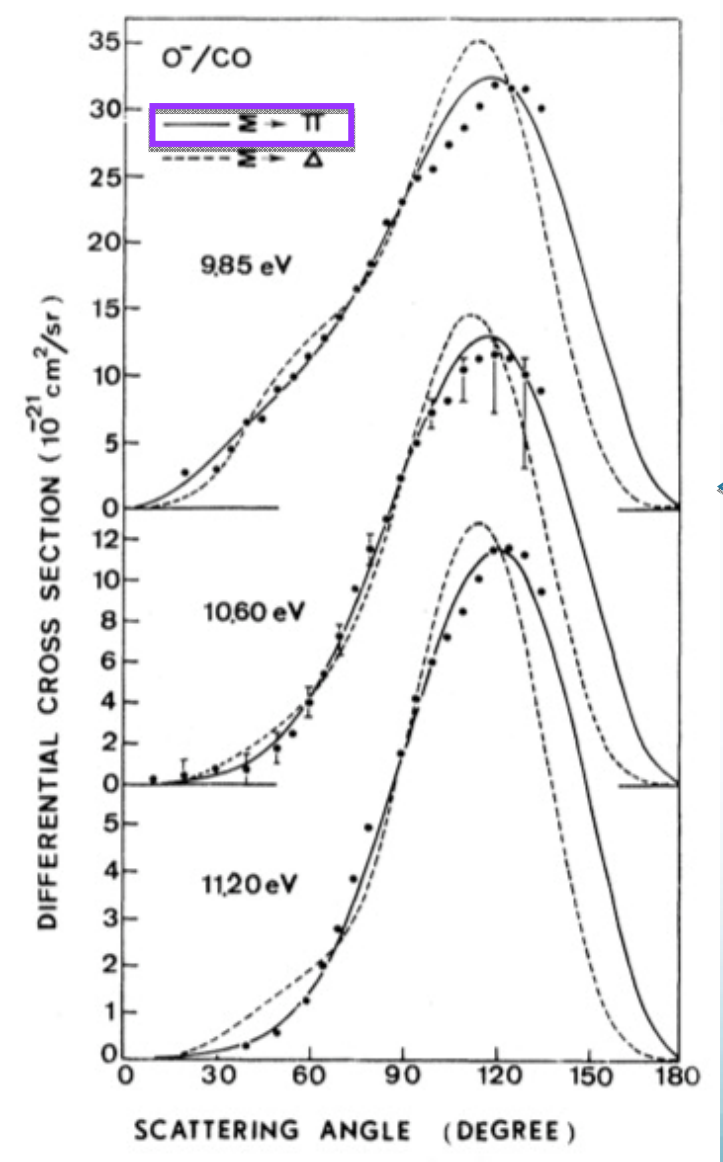
$\mu = \Lambda_f - |\Lambda_i|$

$l \geq |\mu|$

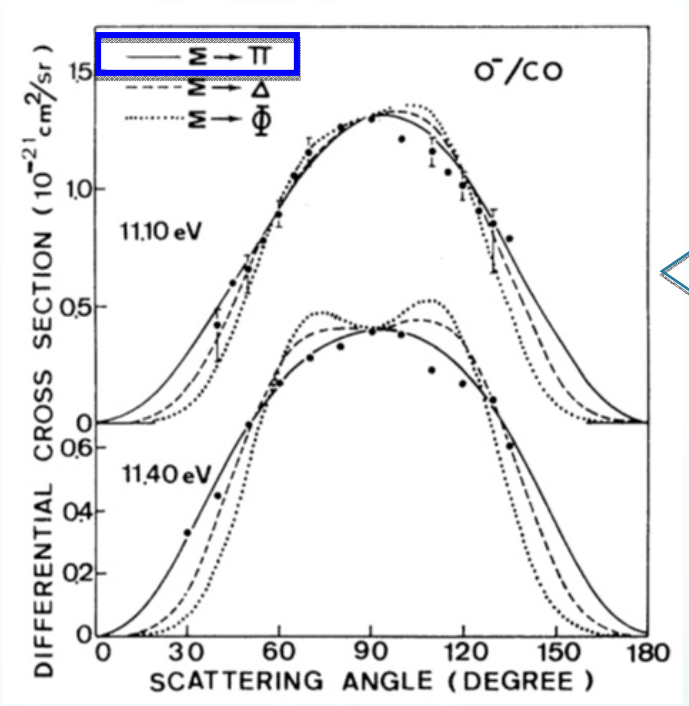
l : even for same parity
odd for opposite parity

$$f(\theta) = A \Big| \sum_{j=0}^{3} a_j e^{i\alpha_j} Y_{j0} \Big|^2 + B \Big| \sum_{k=1}^{4} b_k e^{i\beta_k} Y_{k1} \Big|^2$$

Σ Π



Process I

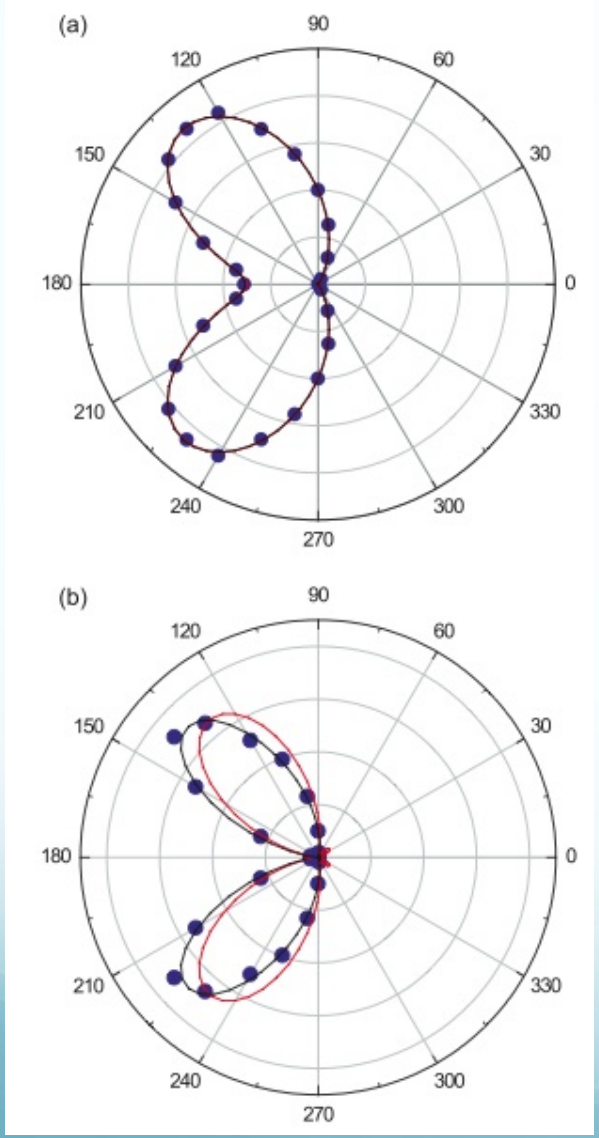


Process II

Hall et al., Phys. Rev. A **15** (1977) 599

Coherent interference in DEA

(Tian et al., PRA **88** (2013) 012708)



10.0 eV

Process I

$\Sigma + \Pi$

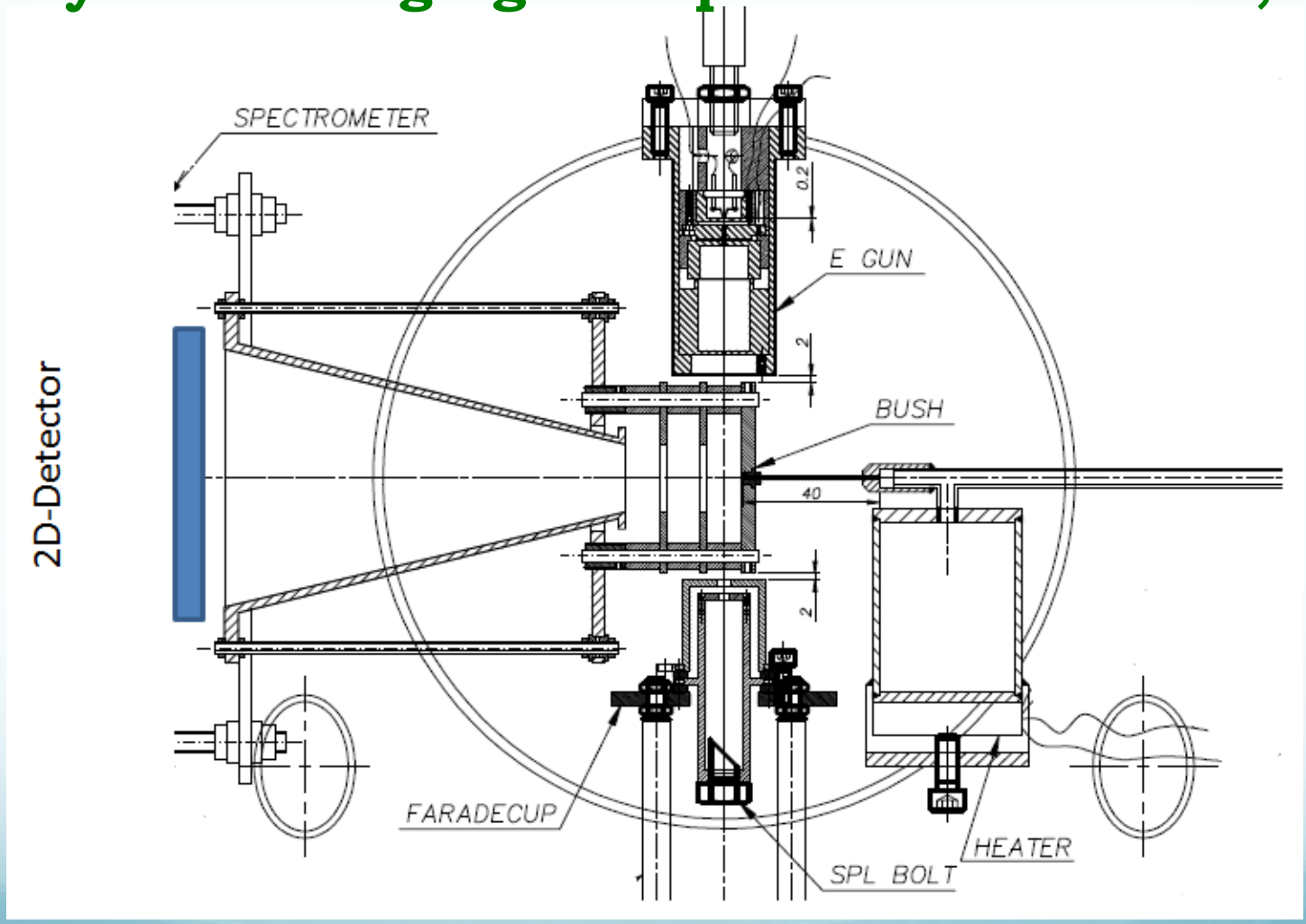
$$f(\theta) = A\left|\sum_{j=0}^{3} a_j e^{i\alpha_j} Y_{j0}\right|^2 + B\left|\sum_{k=1}^{4} b_k e^{i\beta_k} Y_{k1}\right|^2$$

$$\sigma_{\mathrm{DEA}}(k,\Omega) \propto \sum_{\alpha,\beta} I_{\alpha,\beta} + 2\sum_{\alpha\neq\beta} \sqrt{I_\alpha I_\beta}\cos\phi_{\alpha\beta}$$

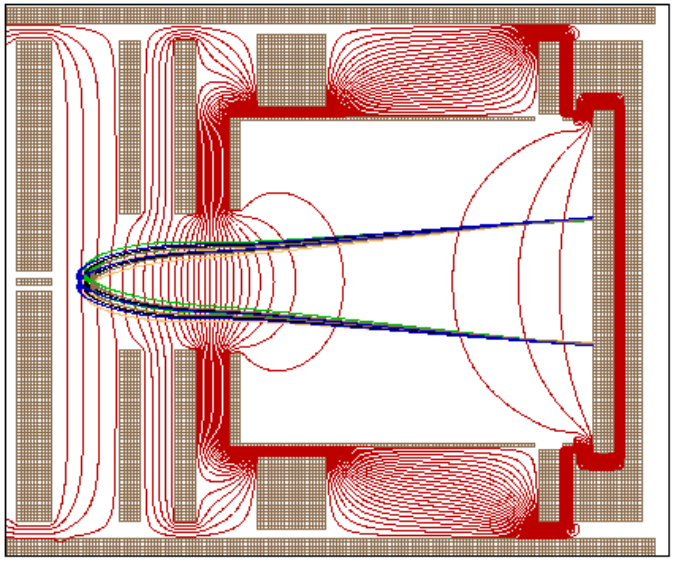
10.6 eV

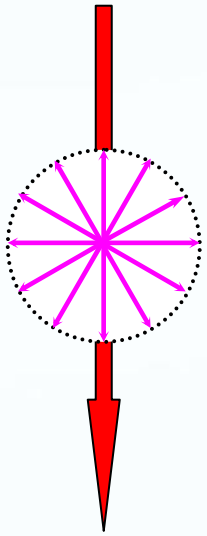
$^2\Pi$, $^2\Delta$, $^2\Phi$

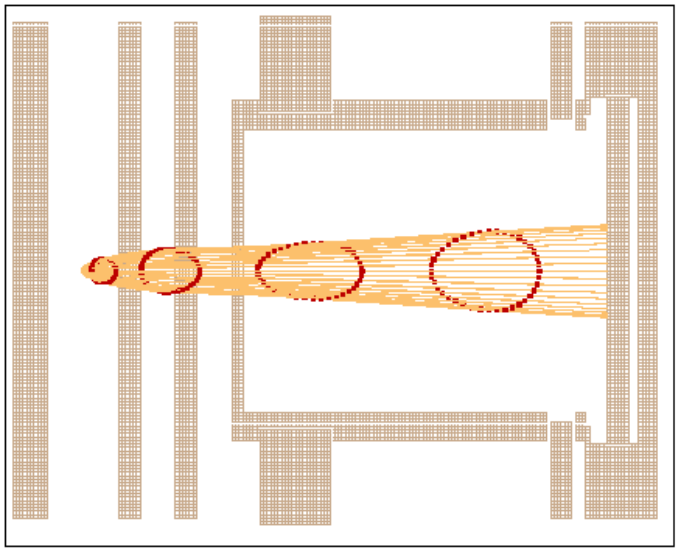
Velocity Slice Imaging set-up at IISER Kolkata, India

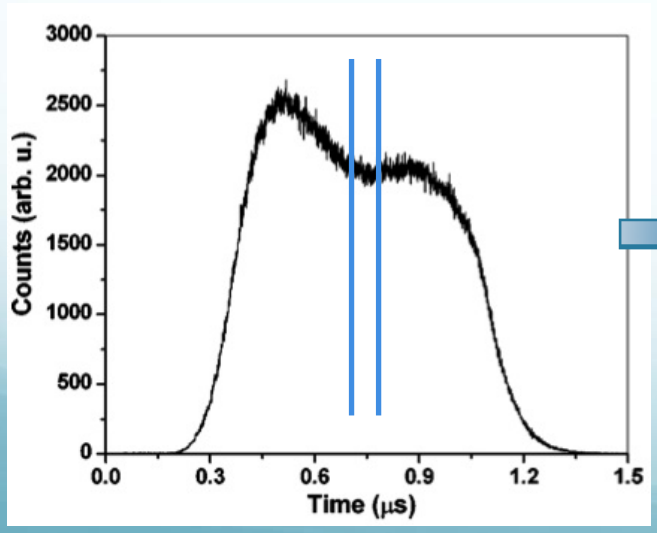


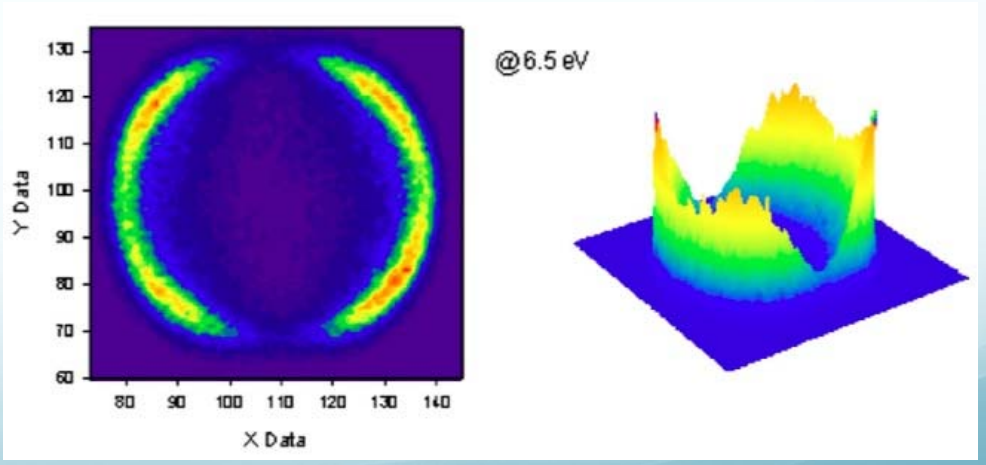
Nag and Nandi, Meas. Sci. Technol. ***26*** *(2015) 095007*





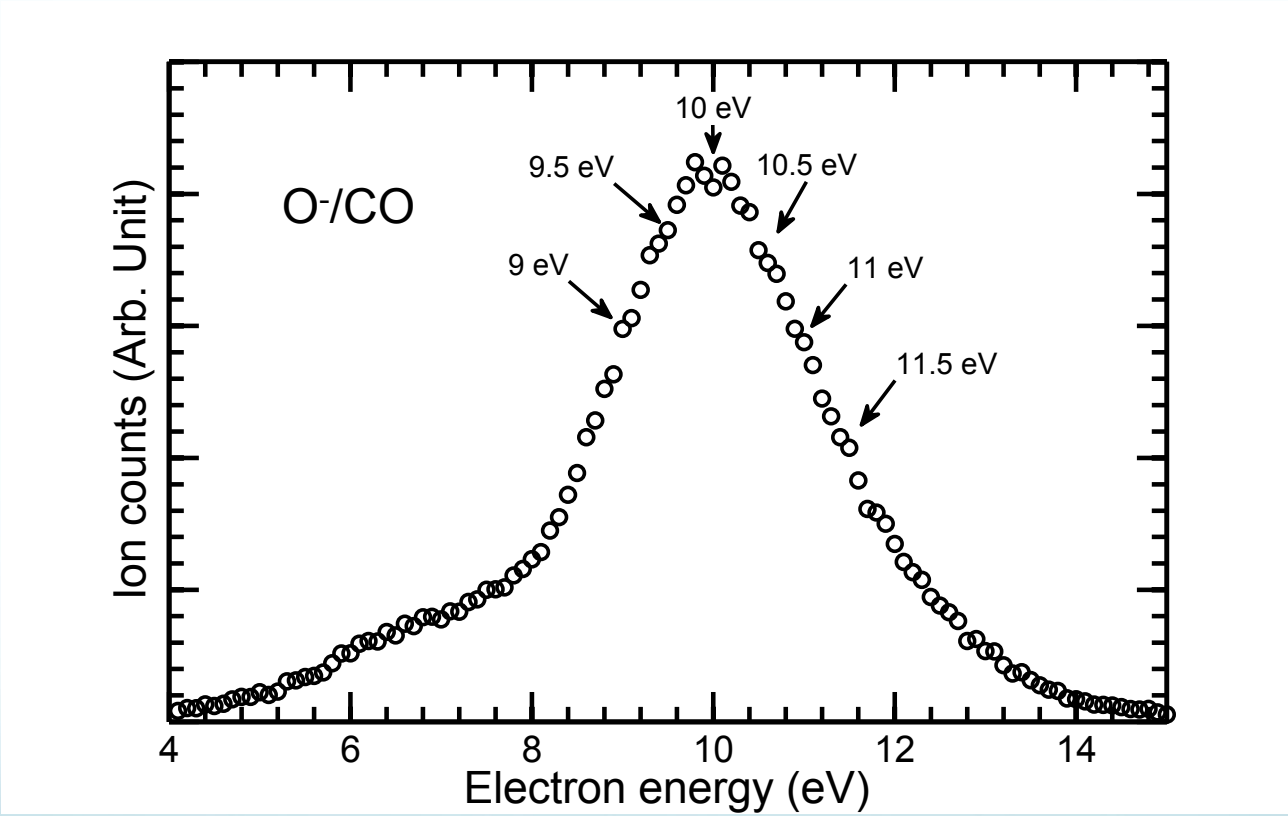






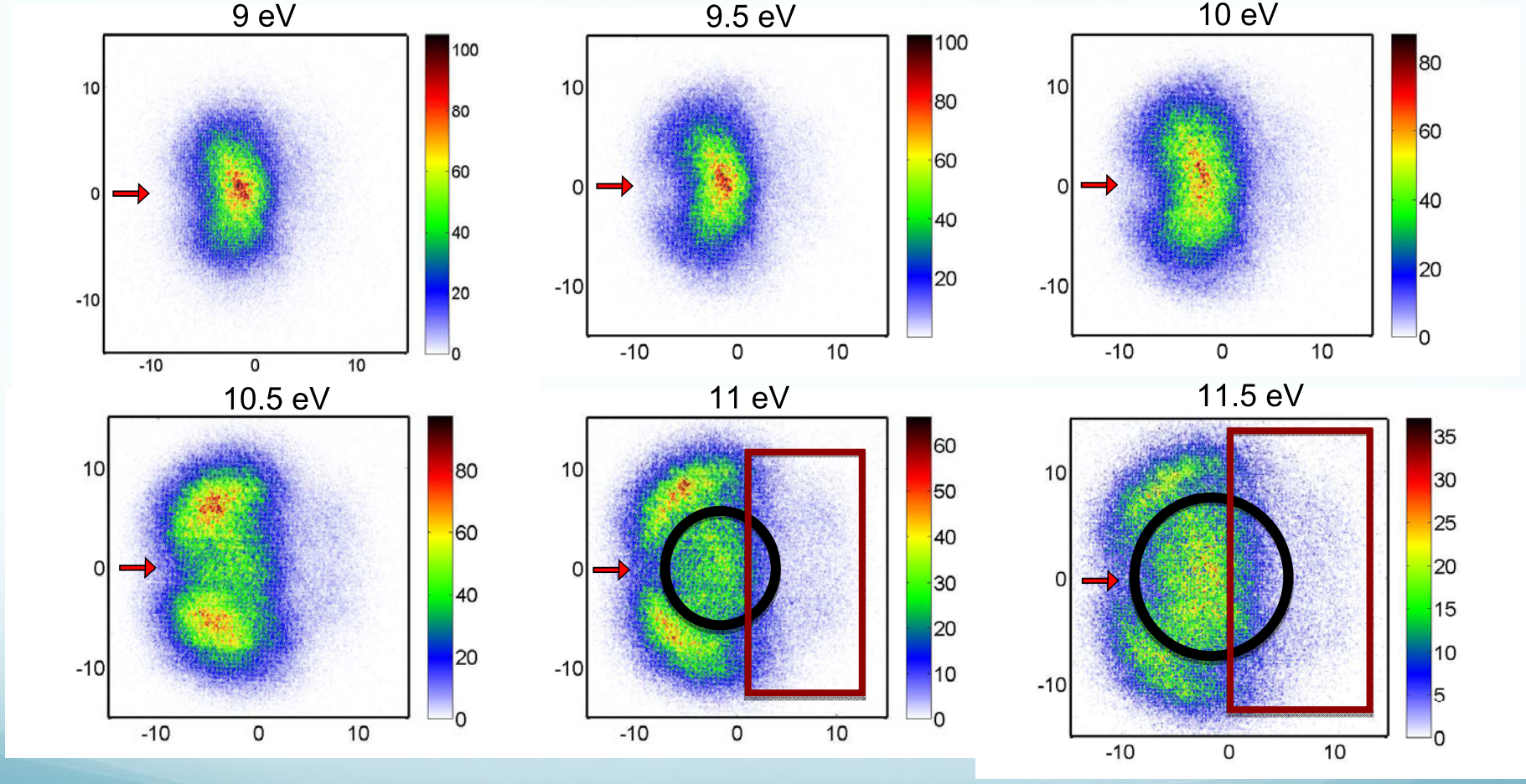
D. Nandi *et al., Rev. Sci. Ins.* ***76*** *(2005) 053107*

Ion Yield Curve



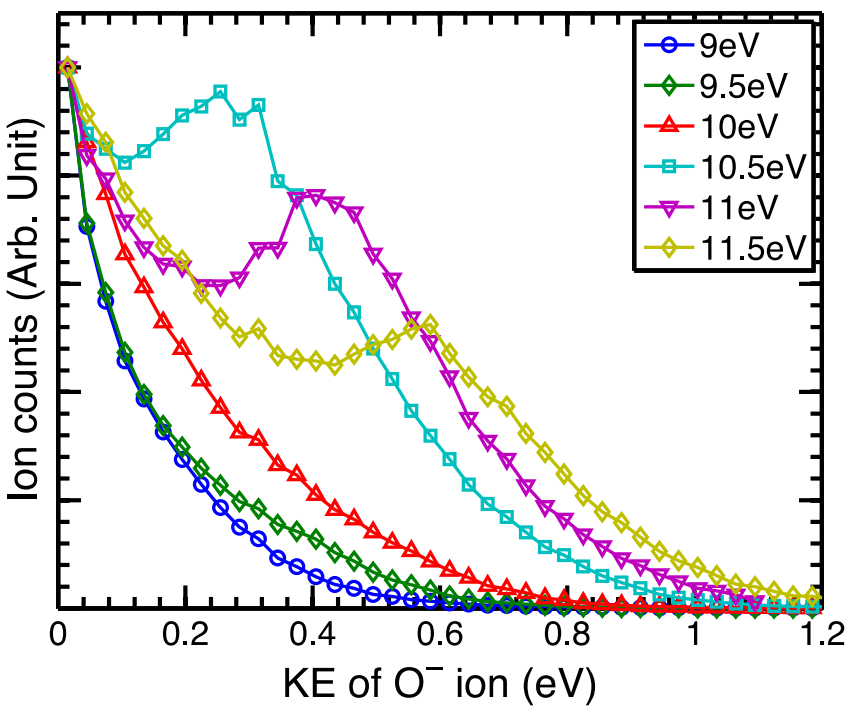
Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130

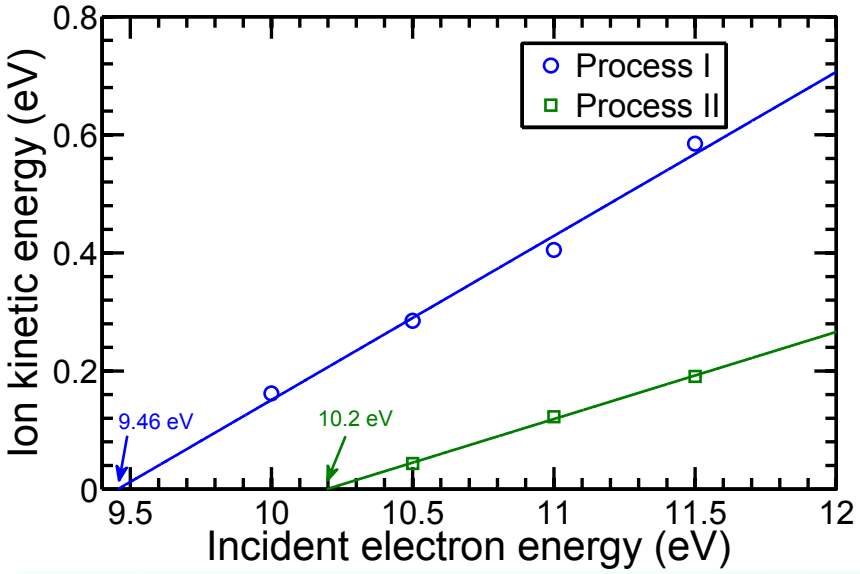
Time Sliced Images of O^-/CO around the Resonance



Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130

Kinetic Energy Distribution





$$E_R = \left(1 - \frac{m}{M}\right)[V_e - (D - A + E^*)]$$

Threshold energy: Process I: 9.62 eV
Process II: 10.88 eV

Experimentally observed:

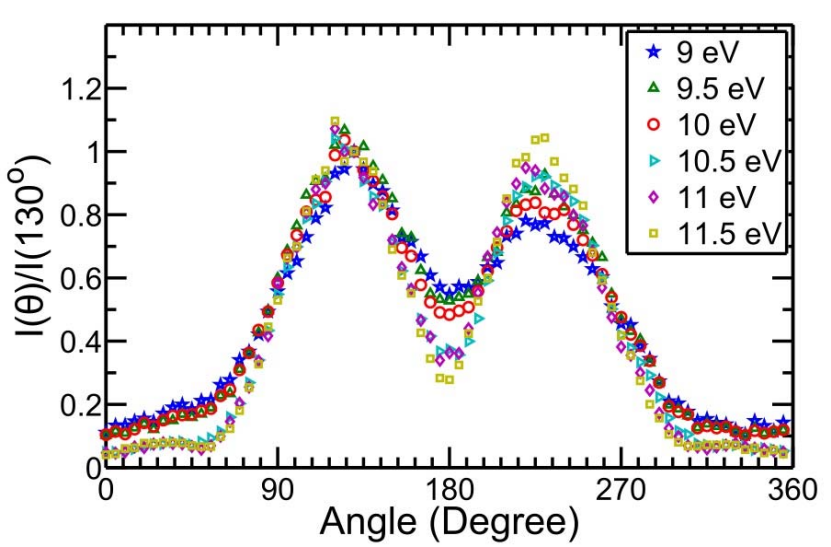
Process I: 9.46 eV

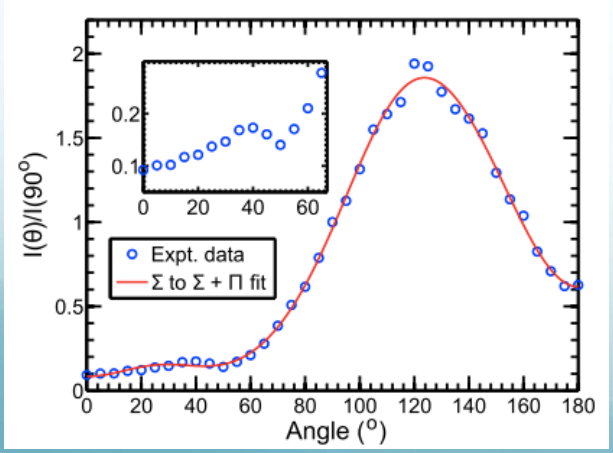
Process II: 10.2 eV

Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130

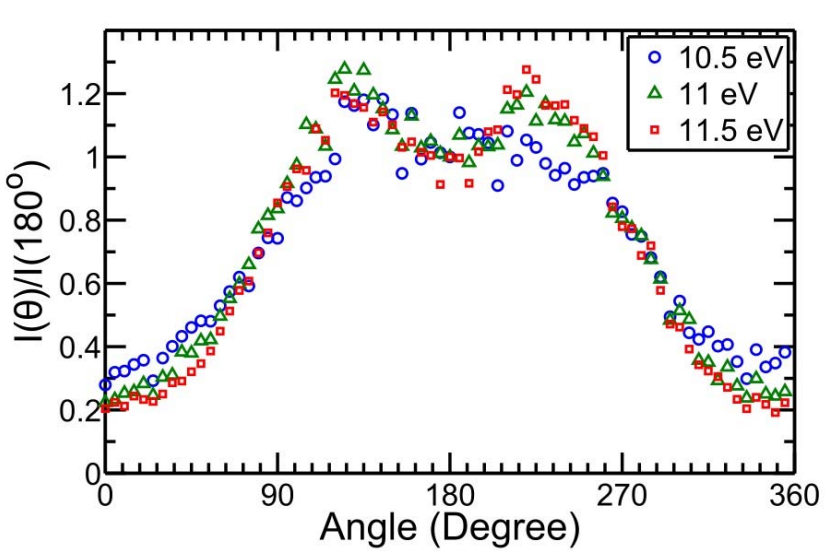
Angular Distribution of O^-/CO at the Resonance

(Process I)



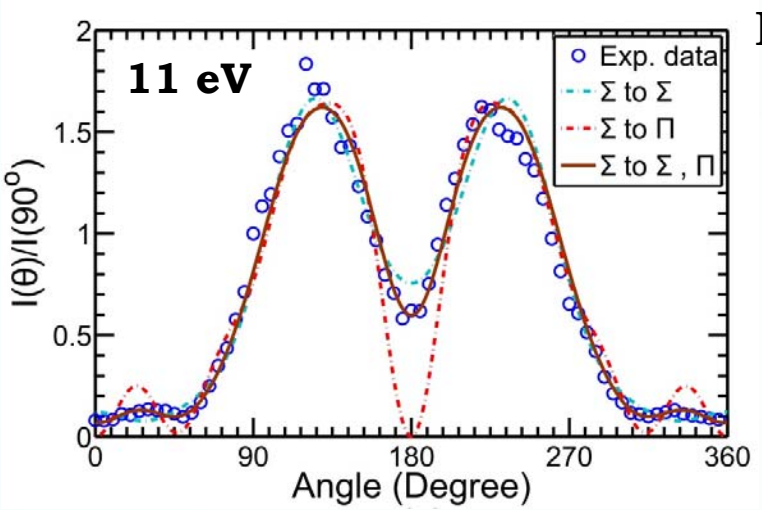


(Process II)



Forward Lobe

Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130



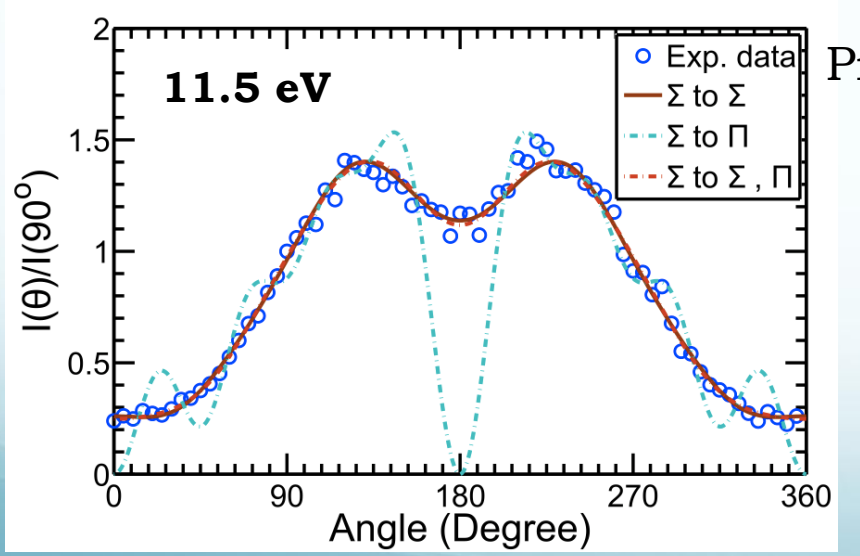
Process I

Axial recoil approximation

$$f(\theta) = A\left|\sum_{j=0}^{3} a_j e^{i\alpha_j} Y_{j0}\right|^2 + B\left|\sum_{k=1}^{4} b_k e^{i\beta_k} Y_{k1}\right|^2$$

Σ Π

✓ Finite cross-section in 0° and 180°



Process II

✓ Forward-backward asymmetry

R-Matrix theory

Dora et al., Eur. Phys. J. D.**70** (2016) 197

Identified $^2\Sigma^+$ resonance

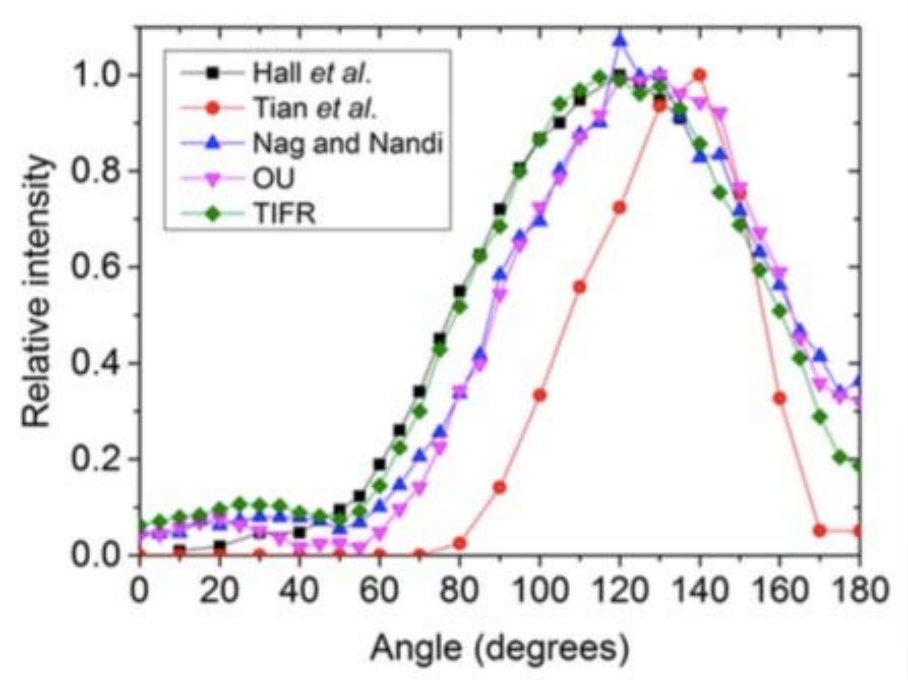
Nag and Nandi, Phys. Chem. Chem. Phys., **17** (2015) 7130

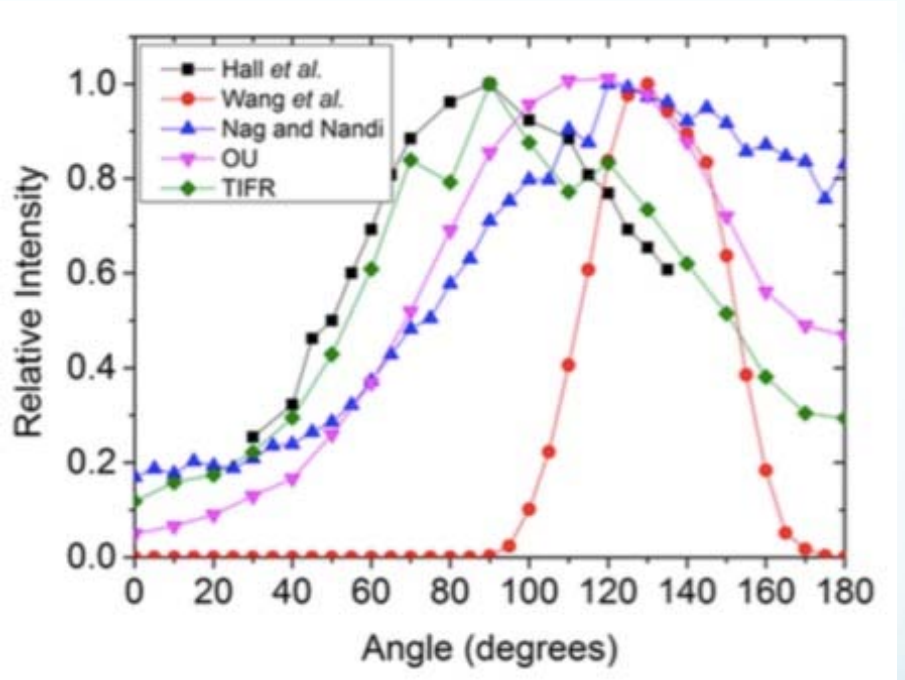
Comparative Study

Process I

K. Gope et al., Eur. Phys. J. D. **70** (2016) 134.

Process II





- Tian et al. : Absence of forward lobe
- Coherent Interference

Incoherent sum of Σ and Π states

Summary/Conclusion

✧ Axial Recoil Approximation VALID

✧ Two overlapping resonances identified.

✧ Process I :: Kinetic energy release is low.

Σ or Σ + Π final state, not only Π state is involved.

✧ Process II :: Kinetic energy release very low!!

Neutral atom (C) in the excited state

Σor Σ + Π final state

✧ **Four partial waves both the cases**

✧ **Interference between partial waves : explained forward-backward asymmetry**

✧ No coherent interference between different states

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