Fully Differential Study of Post-Collision Effects in Ionization of H_2 by Proton Impact

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Quantum-mechanical few-body problem one of the most fundamentally important, unsolved problems in Physics!

Schrödinger equation not solvable for more than two particles, even when underlying forces are precisely known

Dynamic few-body systems like fragmentation processes

Atomic fragmentation particularly suitable because:

- **underlying interaction (electromagnetic) understood**
- **can select systems with small particle number ($\approx 3 - 5$) $\Rightarrow$ kinematically complete exeperiments**

Ionization of H_2 by p impact

Perturbative treatment: expand T in powers of interaction potential V (Born series)

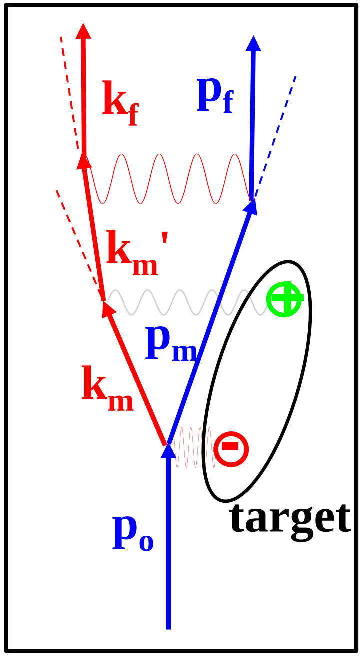
$$T = \langle e^{ik_f r}\,\varphi_f\,|V|\,e^{ik_i r}\,\varphi_i\rangle + \langle e^{ik_f r}\,\varphi_f\,|VG_0V|\,e^{ik_i r}\,\varphi_i\rangle +$$

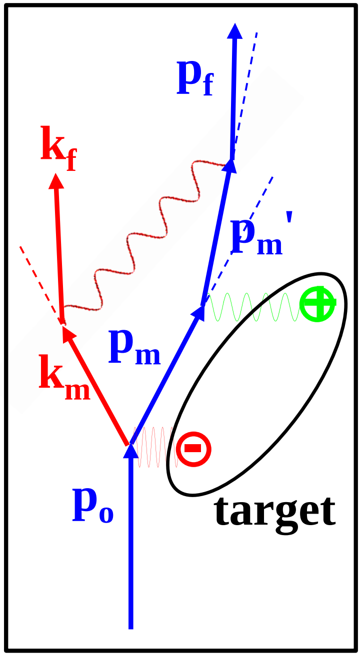
$$\langle e^{ik_f r}\,\varphi_f\,|VG_0VG_0V|\,e^{ik_i r}\,\varphi_i\rangle + \ldots$$

In perturbation theory understanding few-body dynamics means describing relative contributions of higher- vs first-order terms

Particularly important higher-order process: PCI

PE – ET – PE sequence

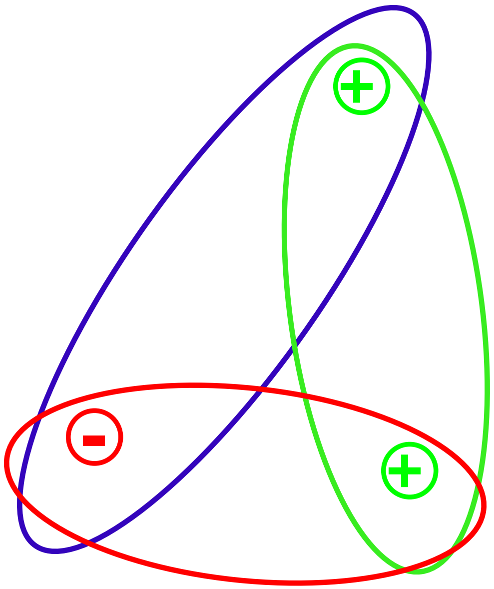




PE – PT – PE sequence

Alternative to Born Series: Distorted wave methods

Higher-order contributions treated in wavefunction of system
Break up three-body system into 3 two-body systems:



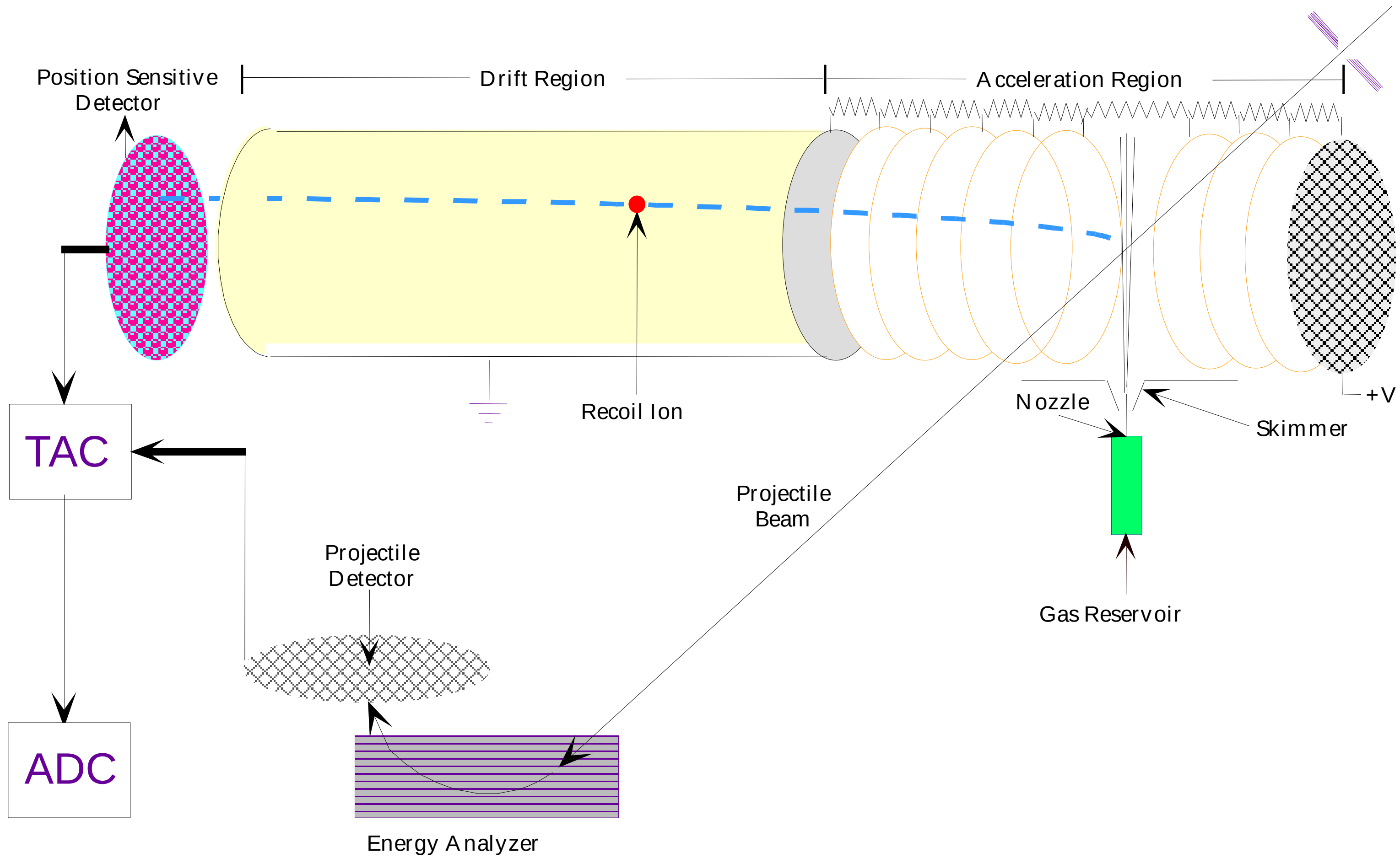
The continuum eigenstate of each two-body subsystem is a (distorted) Coulomb-wave. Approximation: Represent total wavefunction as product of three Coulomb-waves

$$\Psi_f = C_{Pe} C_{PT} C_{Te}$$

Conceptually, all interactions treated to all orders, but 3C wavefunction ignores correlations between particle pairs ⇒ only accurate if one particle far from other two ⇒at small distances none of higher-order terms described accurately

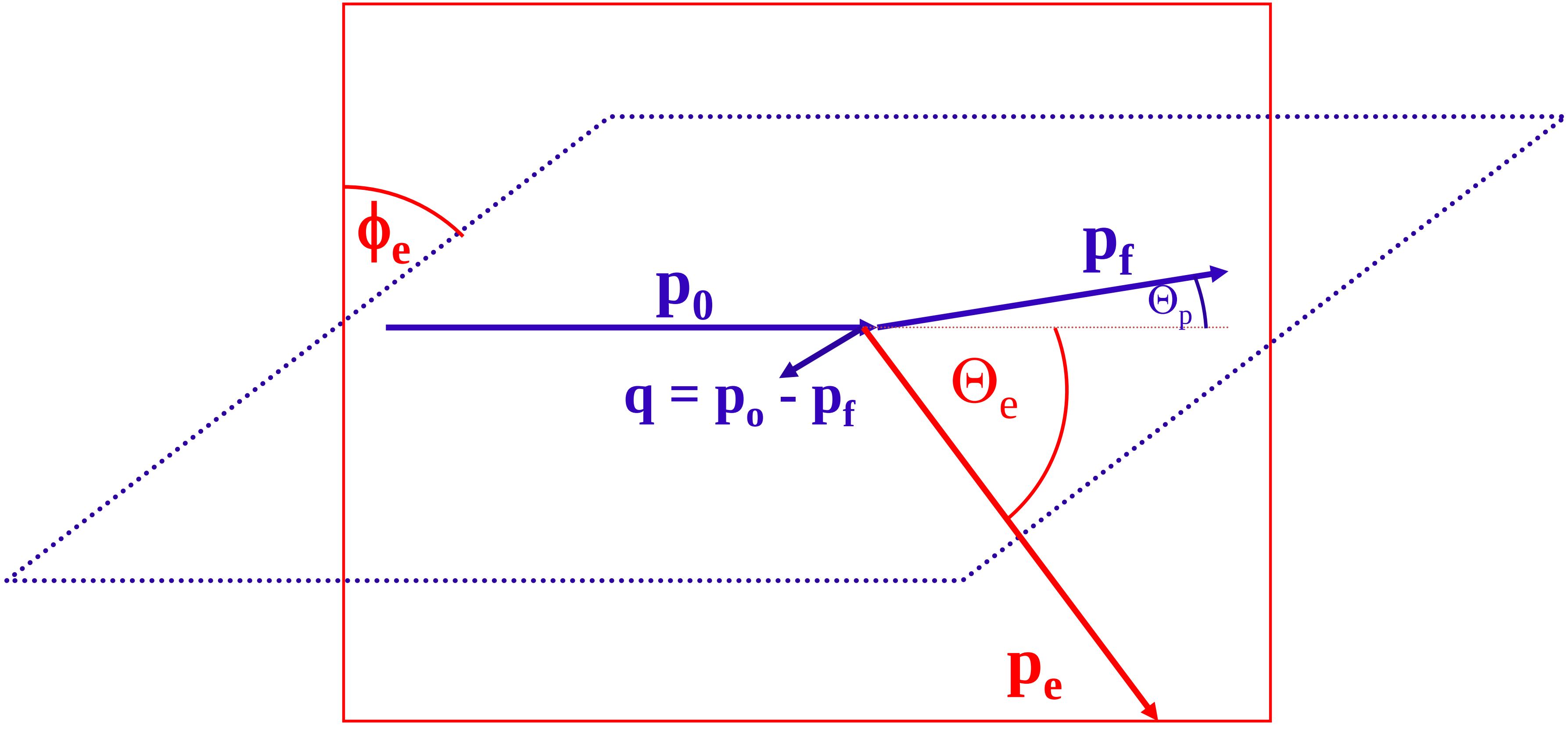
PCI maximizes for $v_{el} = v_p$, no kinematically complete data available!

Experimental Setup, 75 keV p + H_2



Complete projectile and recoil-ion moment measured. Electron momentum from conservation laws ⇒ kinematically complete ⇒ FDCS

Three-Dimensional Fully Differential Single Ionization Data



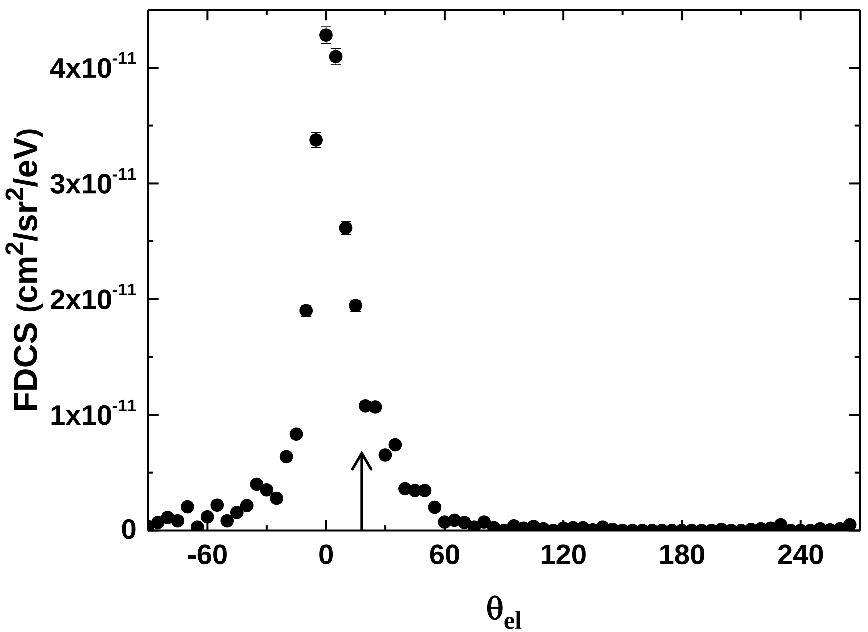
Blue: Scattering plane defined by p_o and p_f

Red: electron emission plane defined by p_o and p_e

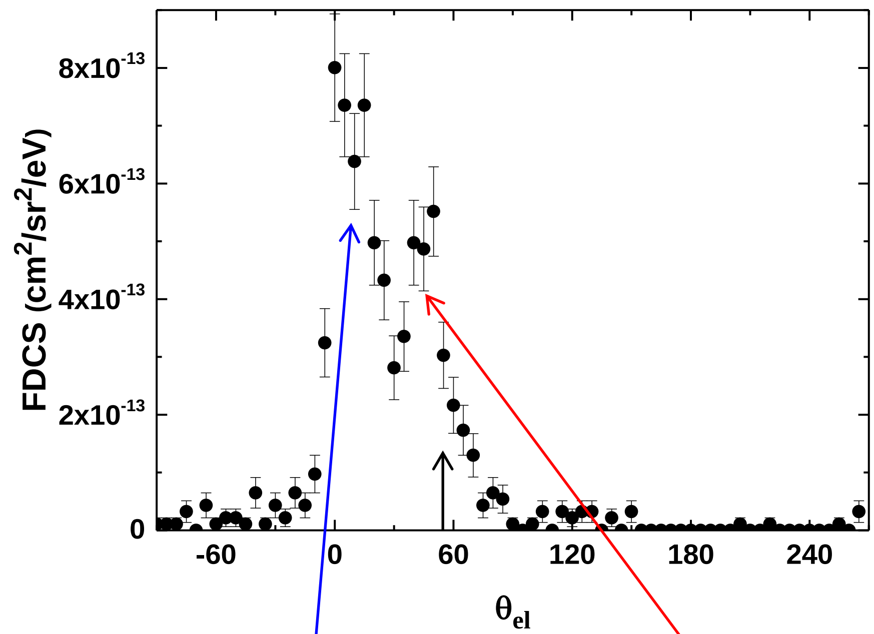
Quantities fixed: $\phi_p = 0$, q, $\phi_e = 0$, and E_e, spectra plotted as a fct. of θ_e

Results: FDCS 75 keV p + H_2

ε = 53 eV, θ_p = 0.1 mrad



ε = 60 eV, θ_p = 0.55 mrad



__small θ_p:__

a) direction of q much closer to $\theta_{el} = 0$

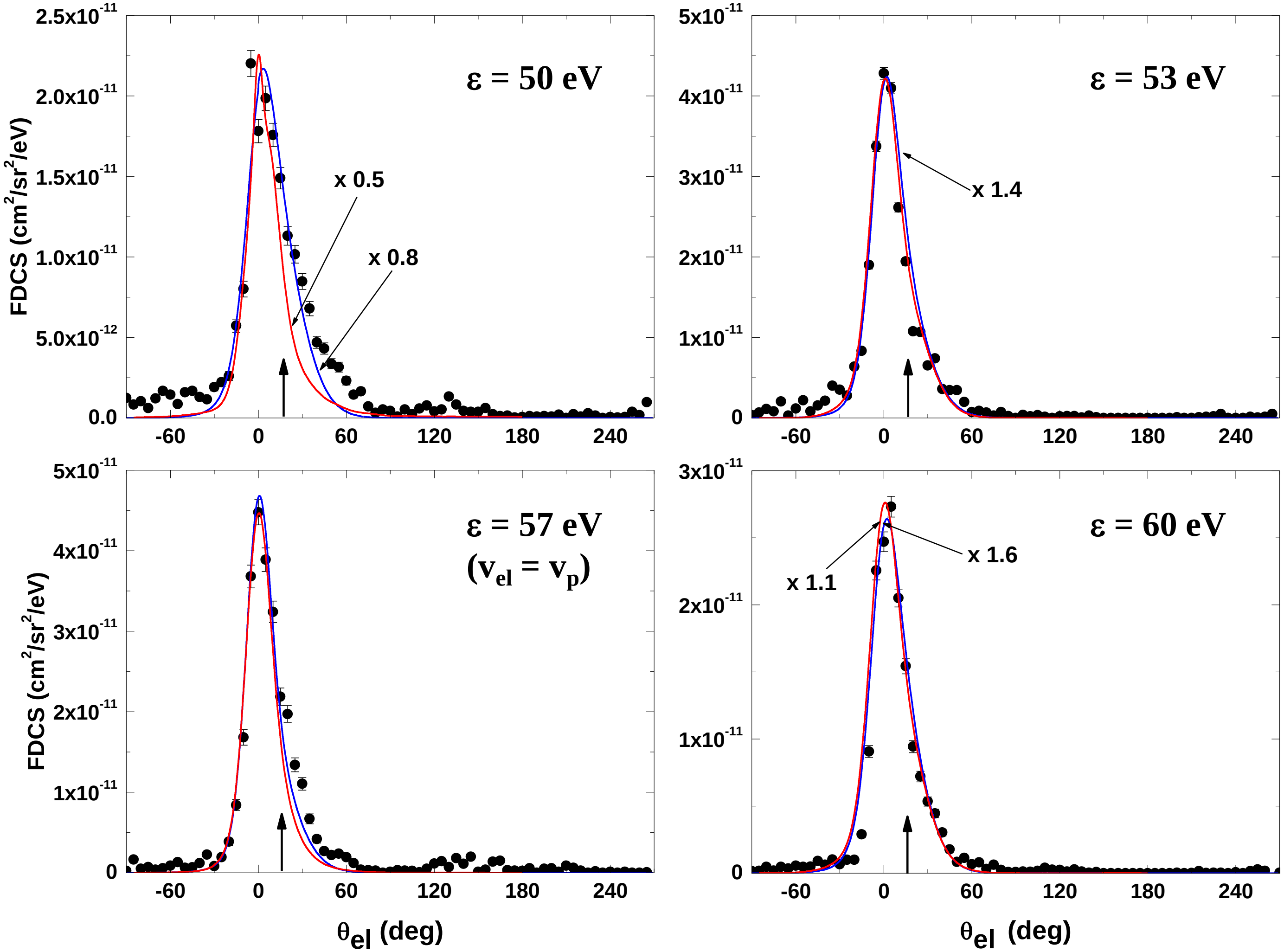
b) binary peak much weaker

$\Rightarrow$ only single peak

„forward peak“ signature of PCI projectile and electron attract each other towards beam axis

„binary peak“ signature of 1st order process momentum conservation: near θ_q

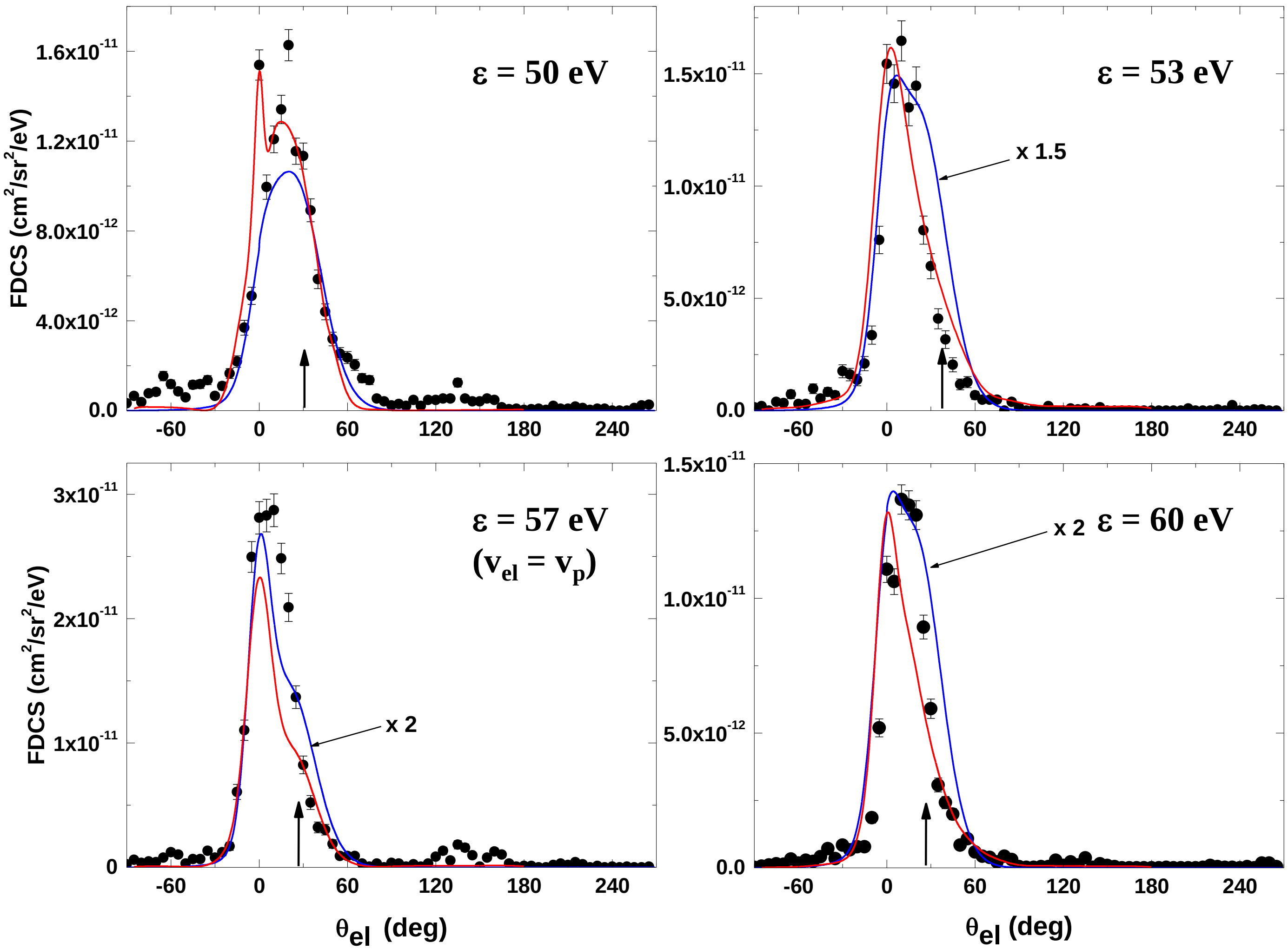
FDCS for θ_p = 0.1 mrad



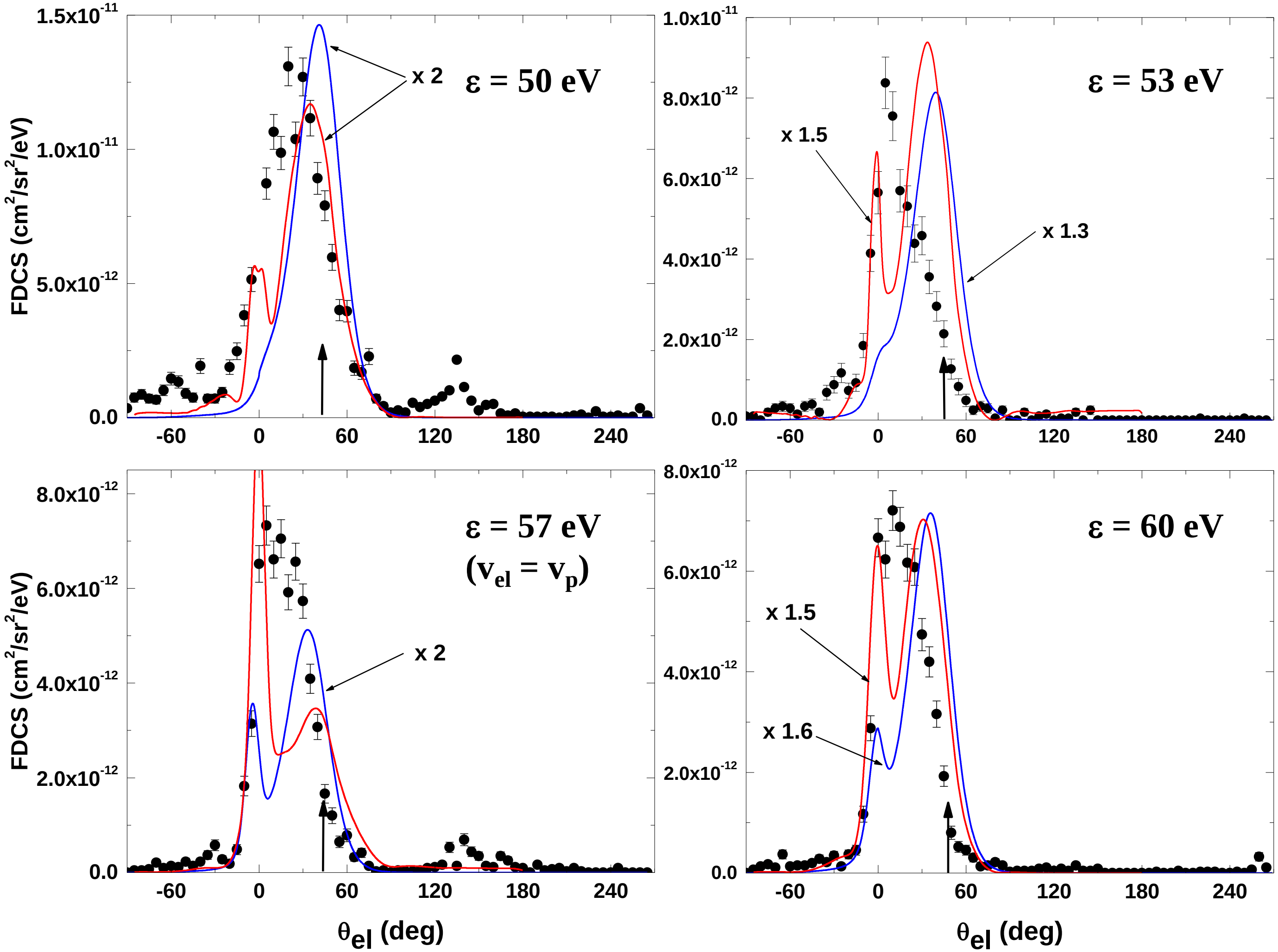
Red curves: 3DW model

Blue curves: CDW-EIS model

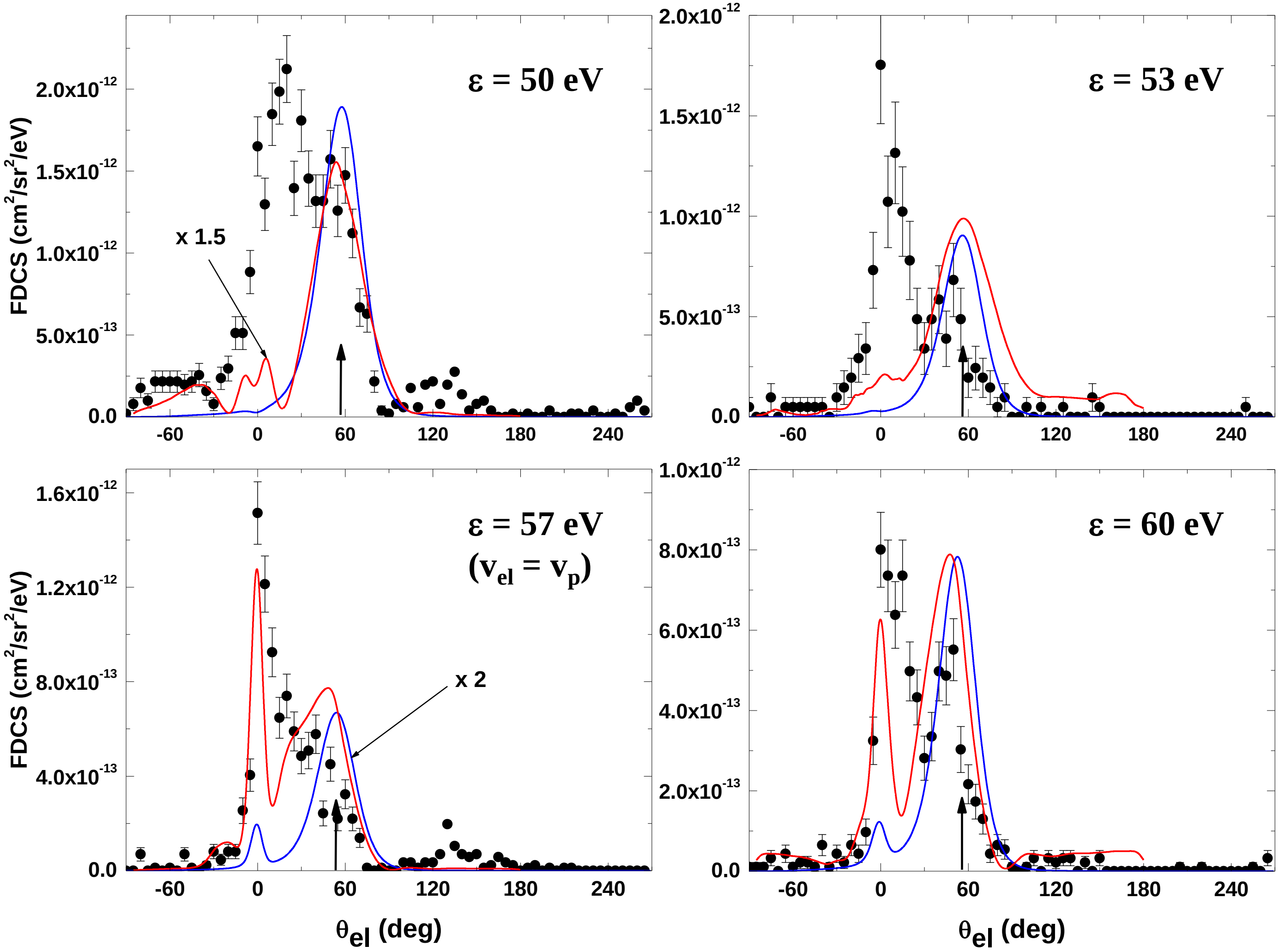
$\theta_p = 0.2$ mrad



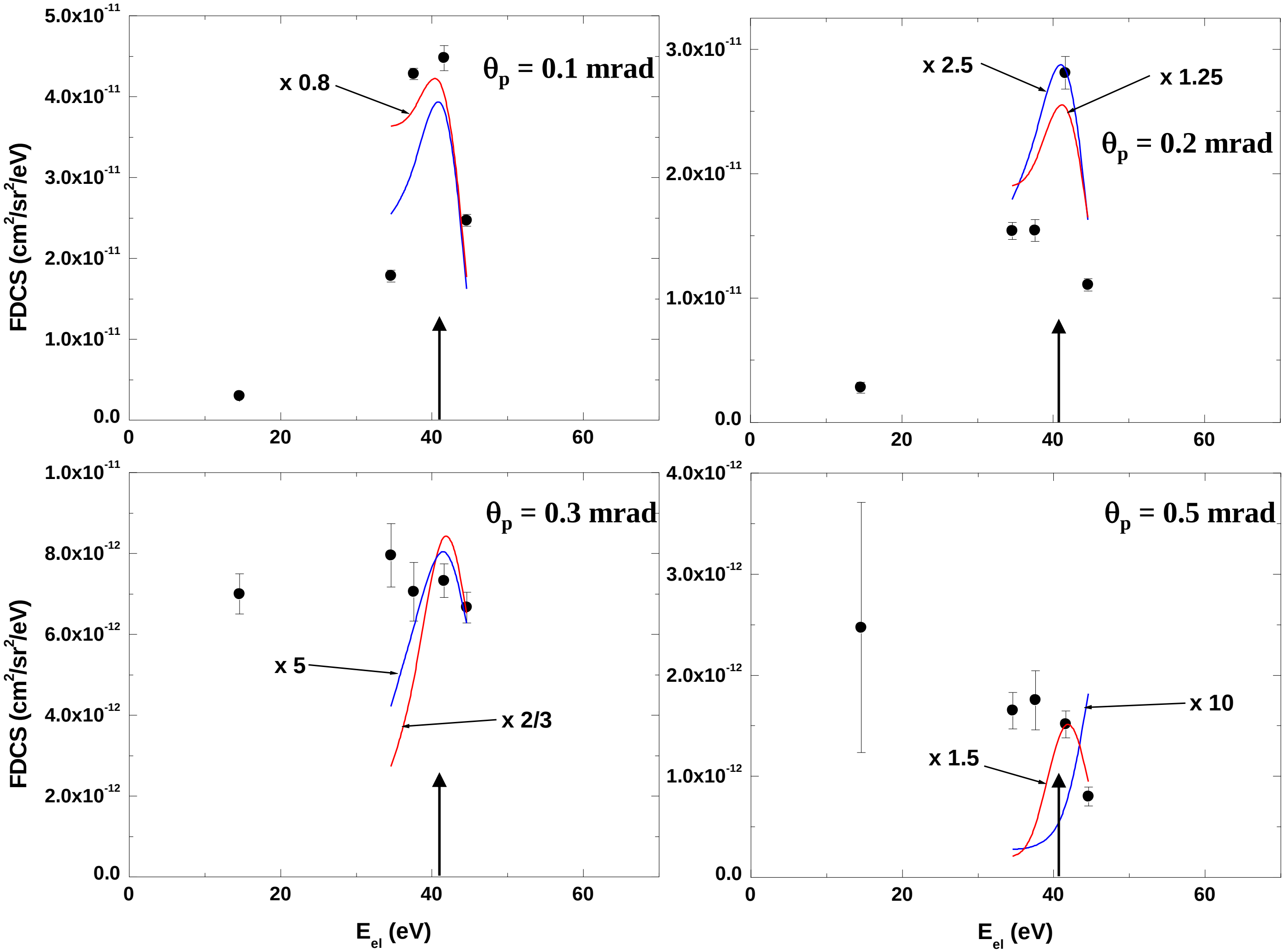
θ_p = 0.325 mrad



θ_p = 0.55 mrad



Energy-dependence of FDCS for $\theta_e = 0^o$



$\Rightarrow$ **Large discrepancies between experiment and between two conceptually very similar theoretical models!**

At small electron energies much smaller discrepancies and theories agree with each other $\Rightarrow$ at velocity matching FDCS particulalrly sensitive to details of few-body dynamics!

<u>Possible causes for discrepancies:</u>

a) PT interaction not accurate in theory
3C wavefunction only accurate if at least 1 particle far from other 2. PE – PT – PE sequence selects events where all 3 particles are close to each other

b) Capture channel not included in theory $\Rightarrow$ due to unitarity capture is erroneously counted as ionization in transition amplitude

c) Projectiles treated as fully coherent waves, but in reality due to intrinsic momentum spread coherence length is finite

⇒ What type of theory is needed?

a) non-perturbative because slow projectiles cannot be regarded as small perturbation ⇒ large basis set needed

b) should incorporate two-center basis set including bound projectile states to account for capture

c) projectiles should be described by wave packet with a width reflecting the coherence length

Non-perturbative models with two-center basis sets for ion impact have been developed recently (Kadyrov et al., Walters et al., Pindzola et al.). First results on FDCS for H_2 can be expected soon.

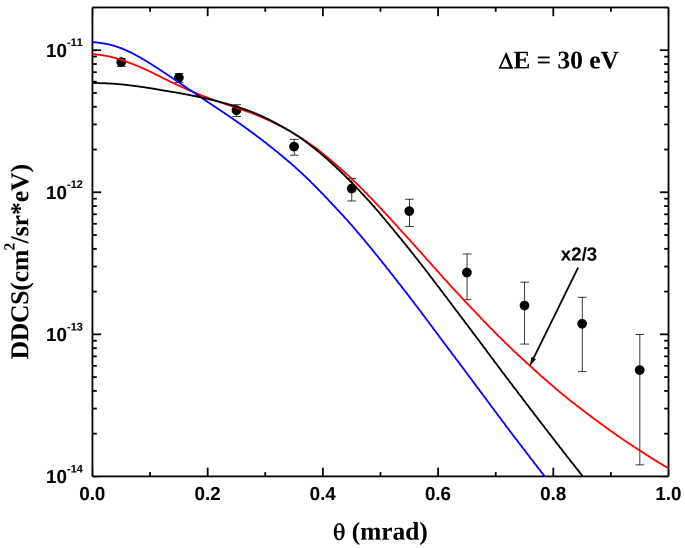
Incorporating wave packets in such models very challenging

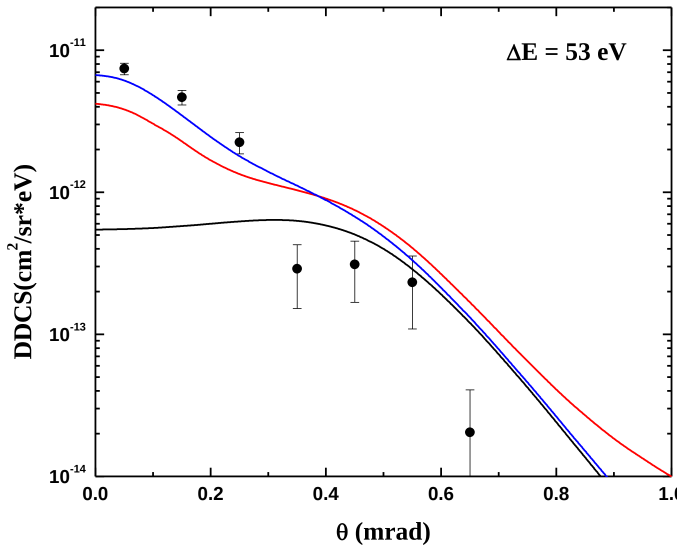
Conclusions

- **Fully differential cross sections for ionization in 75 keV p + H_2 measured.**
- **Major discrepancies between experiment and theory and between two conceptually very similar models.**
- **At matching velocity FDCS very sensitive to details of few-body dynamics.**
- **Potential problems with perturbative methods:**
  a) capture not included
  b) 3C wavefunction not accurate when all particles close
  c) projectile coherence not realistically described
- **What is needed: non-perturbative calculations with two-center basis set and wave packet describing projectile.**

SBA-2C:

Black: FBA
no PCI
Blue:
only PE-ET-PE
Red: PE-ET-PE
and PE-PT-PE





⇒ PE – ET – PE sequence dominant PCI channel in SBA-2C

CDW-EIS:

Black: FBA
no PCI
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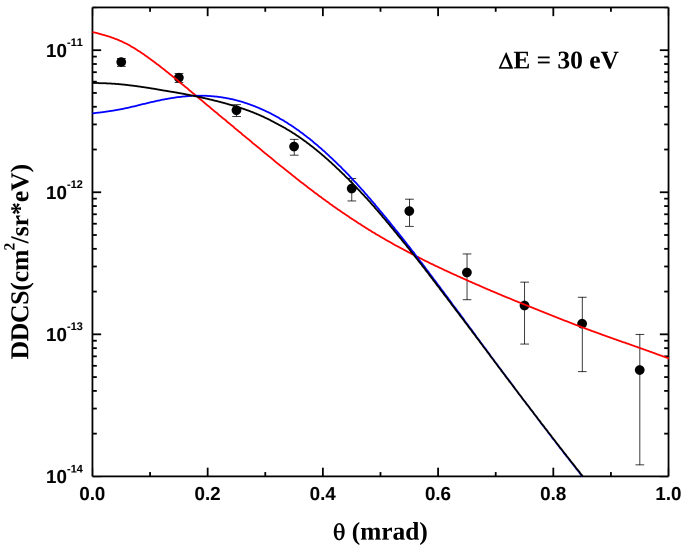
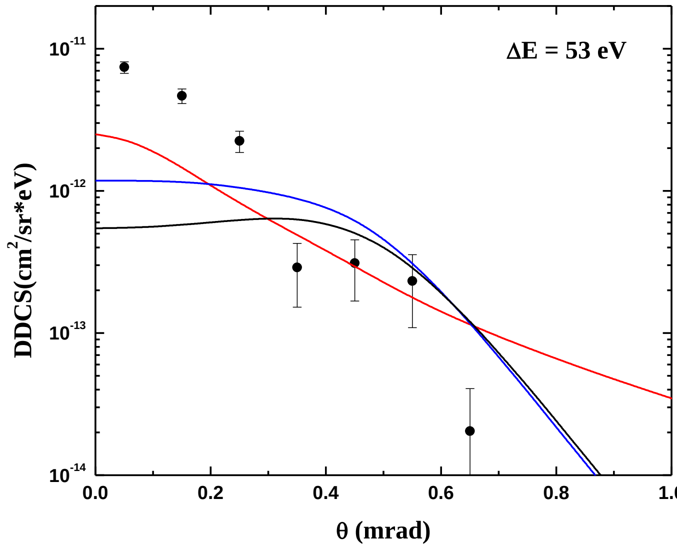
and PE-PT-PE





⇒ PE – PT – PE sequence dominant PCI channel in CDW-EIS