

# Photoelectron Circular Dichroism (PECD): conformer selectivity and induced chirality

**Etienne Rouquet**, <sup>a,b</sup> **Madhusree Roy Chowdhury**, <sup>b</sup> **Gustavo Garcia**, <sup>b</sup> **Laurent Nahon**, <sup>b</sup> **Jennifer Dupont**, <sup>a</sup> **Valéria Lepère**, <sup>a</sup> **Katia Le Barbu-Debus**, <sup>a</sup> **Anne Zehnacker** <sup>a</sup>

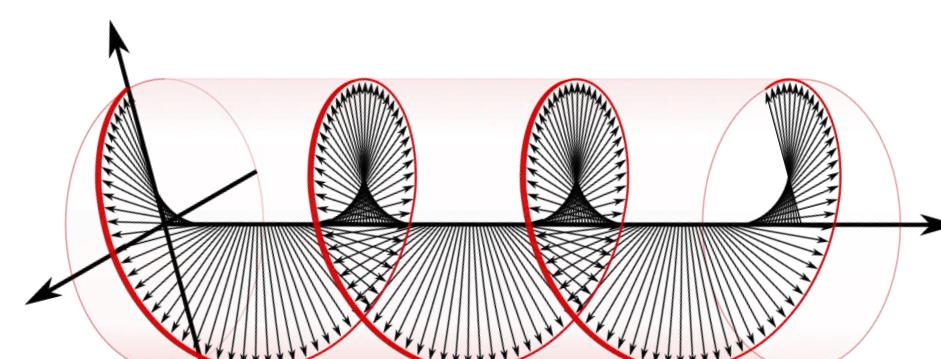
**a) Institut des Sciences Moléculaires d'Orsay (ISMO), 91405 Orsay, France**

**b) Synchrotron SOLEIL, 91190 Saint-Aubin, France**

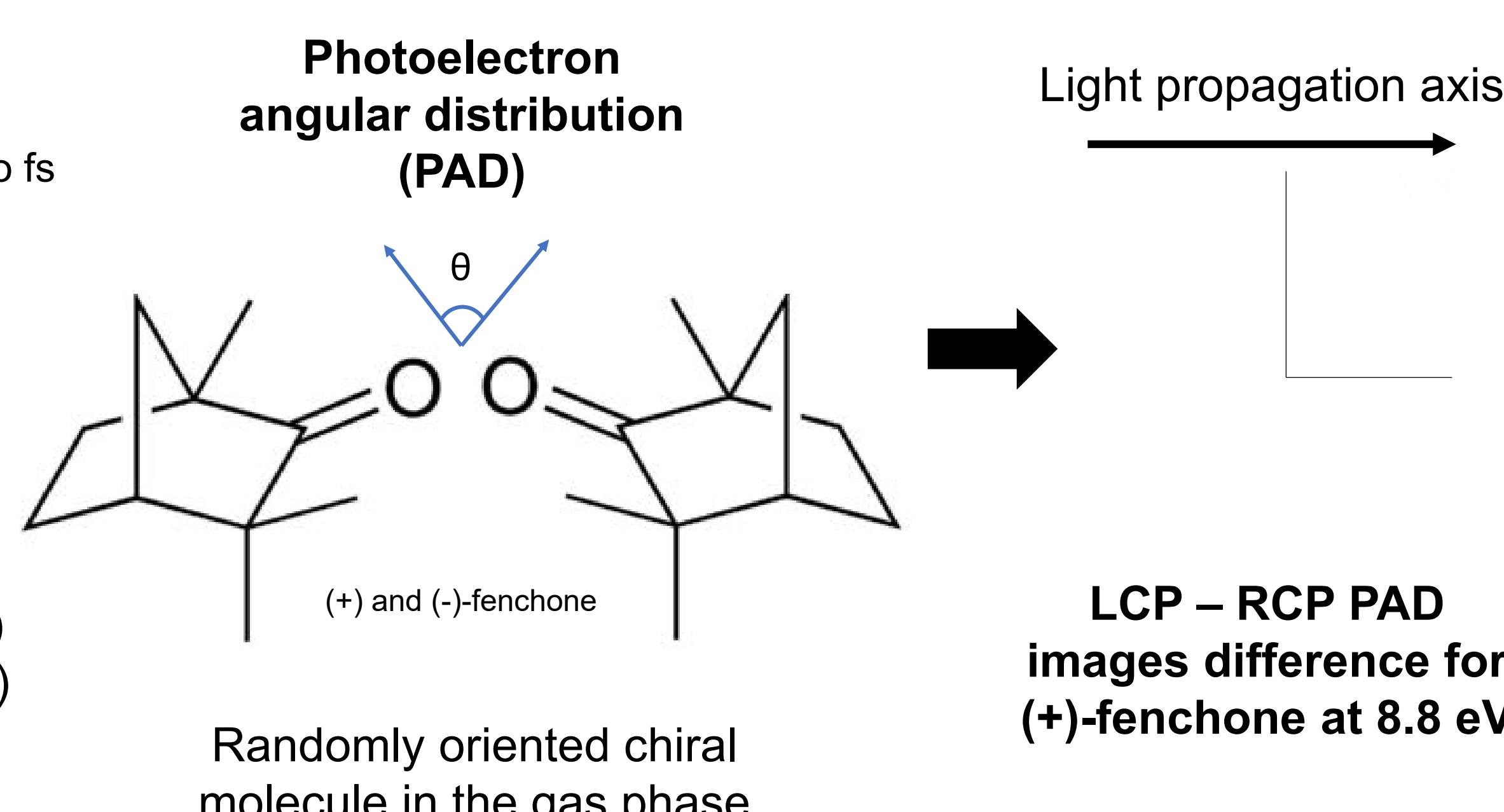
## Photoelectron Circular Dichroism (PECD)

Photoionization process, either:

- One-photon ionization (synchrotron radiation)
- Multi-photon ionization (ns to fs laser setups)



Circularly polarized light (CPL)  
Right or Left helicity (RCP/LCP)



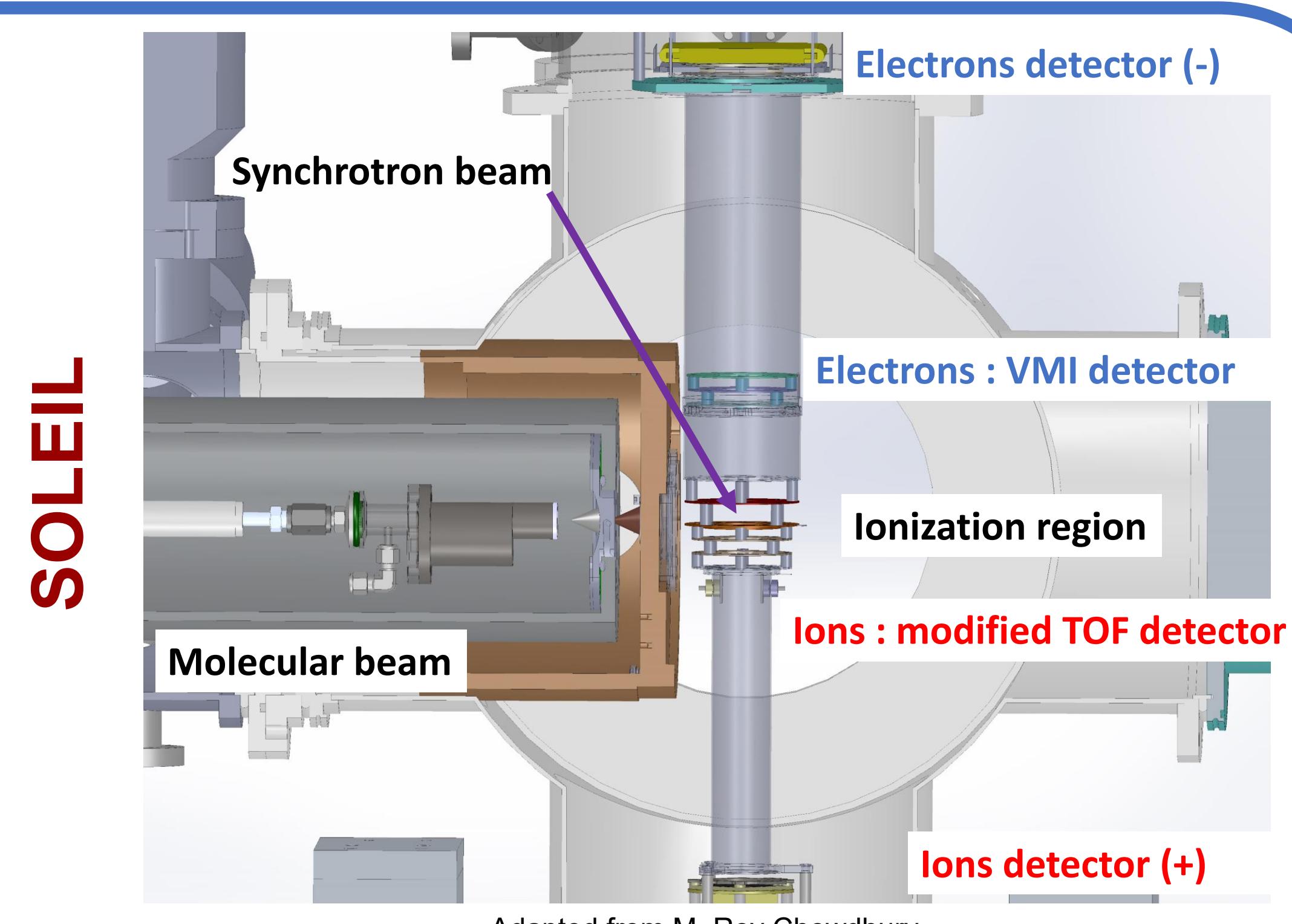
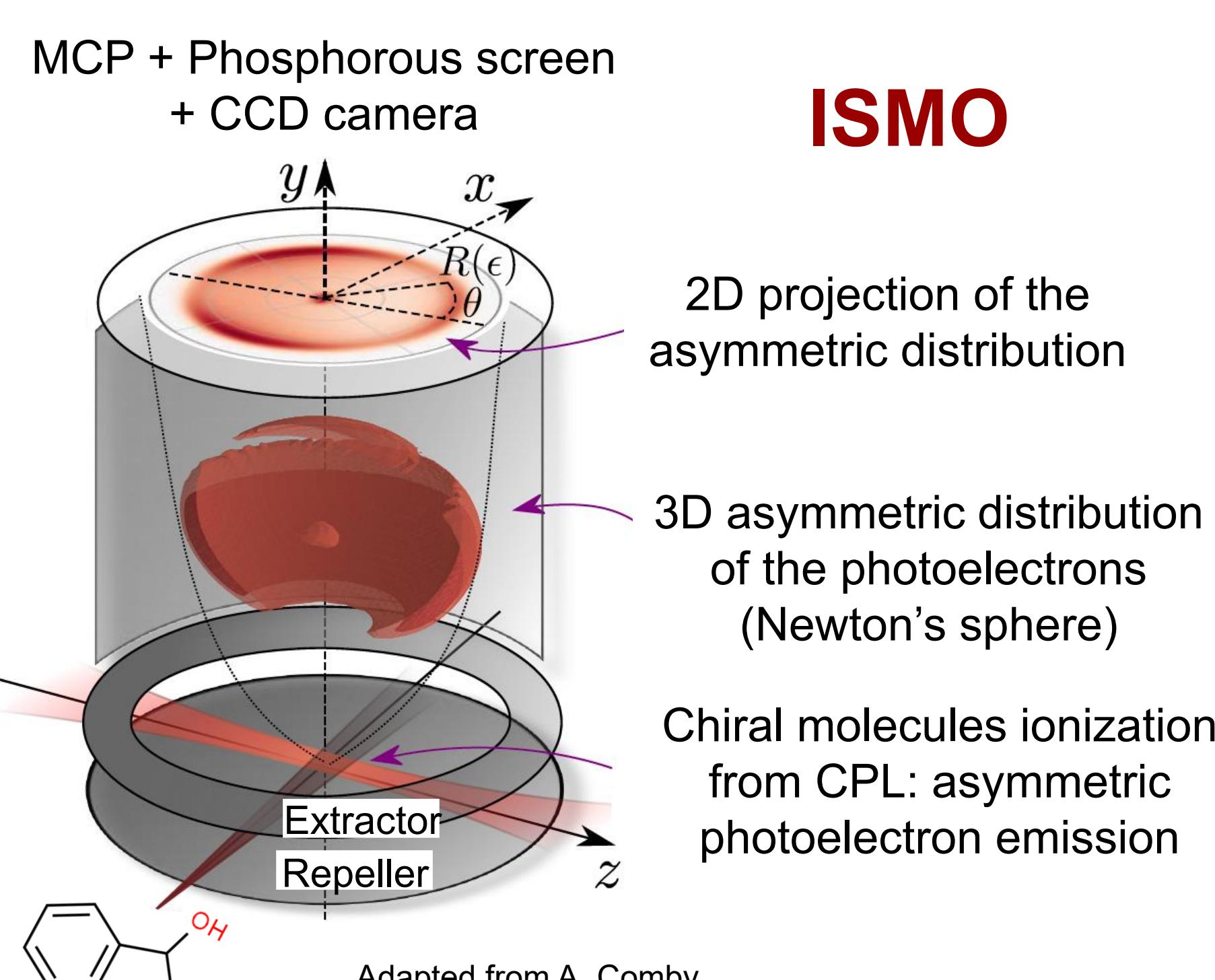
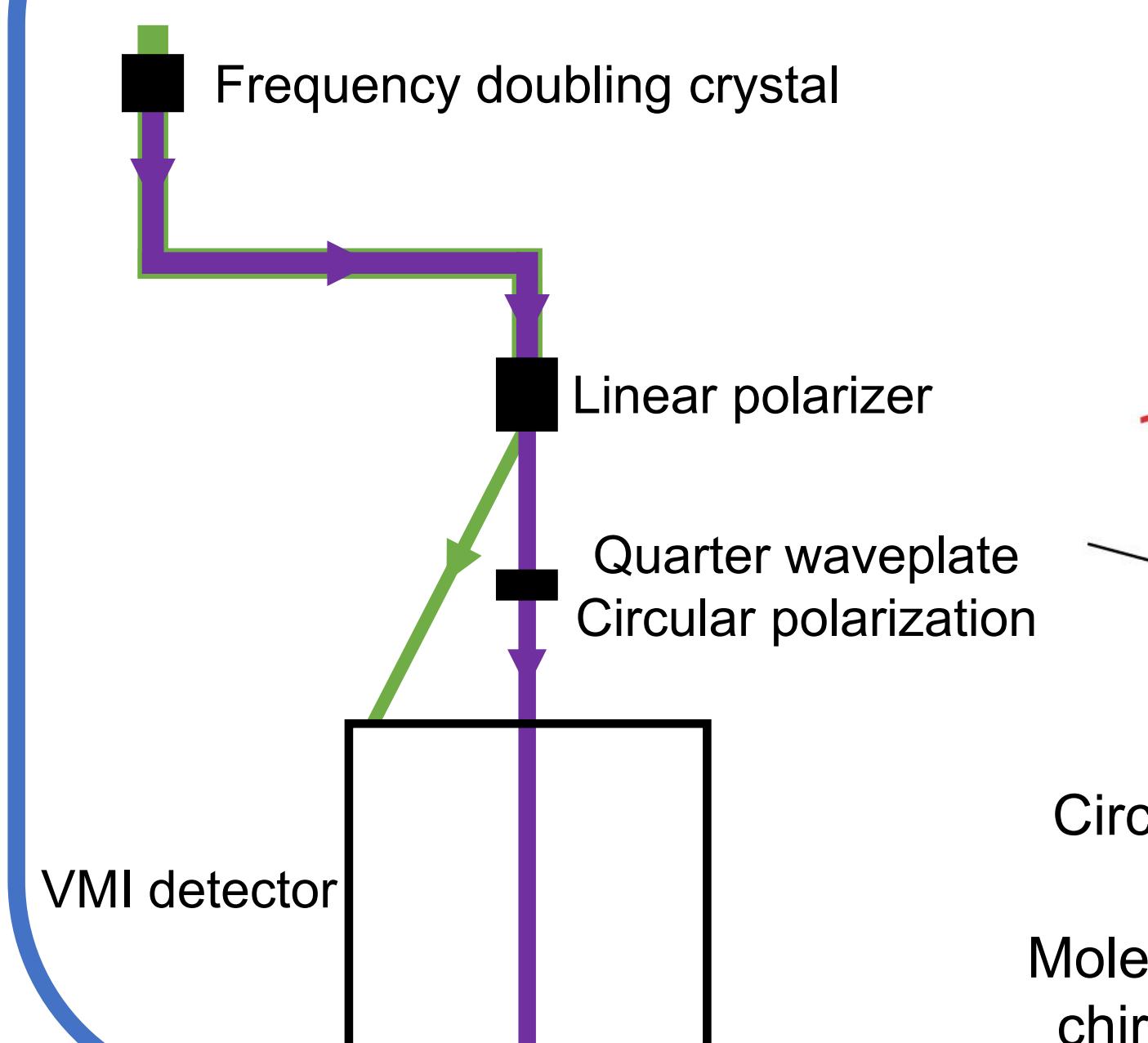
**PECD: Forward/backward asymmetry** with respect to the light propagation axis in the PAD, after ionization of a chiral molecule by a CPL

Allowed in the dipole approximation → strong effect (highest PECD value recorded: **40,7%**)

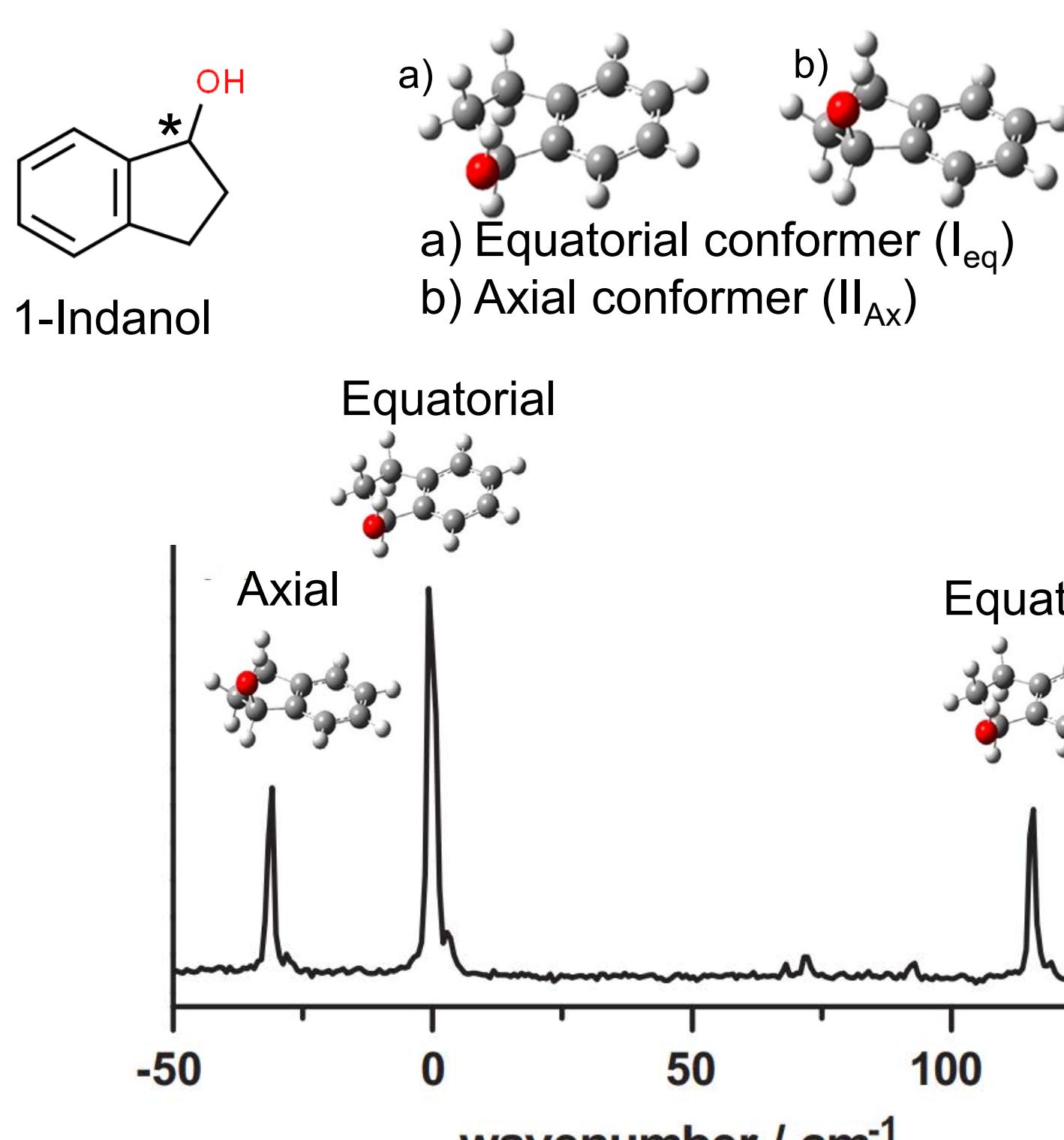
- Allows for **absolute configuration** and **e.e. determination**
- Fine sensitivity to the molecular potential: **complexation, clustering, conformation, isomers, vibration etc...**
- **Sensitivity to the initial state** (orbital of origin) and **final state** (scattering process, kinetic energy dependent)

To see more : L. Nahon et al. (2015) *J. Electron. Spectrosc. Relat. Phenom.* **204**, 322  
R. Hadidi et al. (2018) *Adv. Phys.:X* **3**:1

## Experimental setups

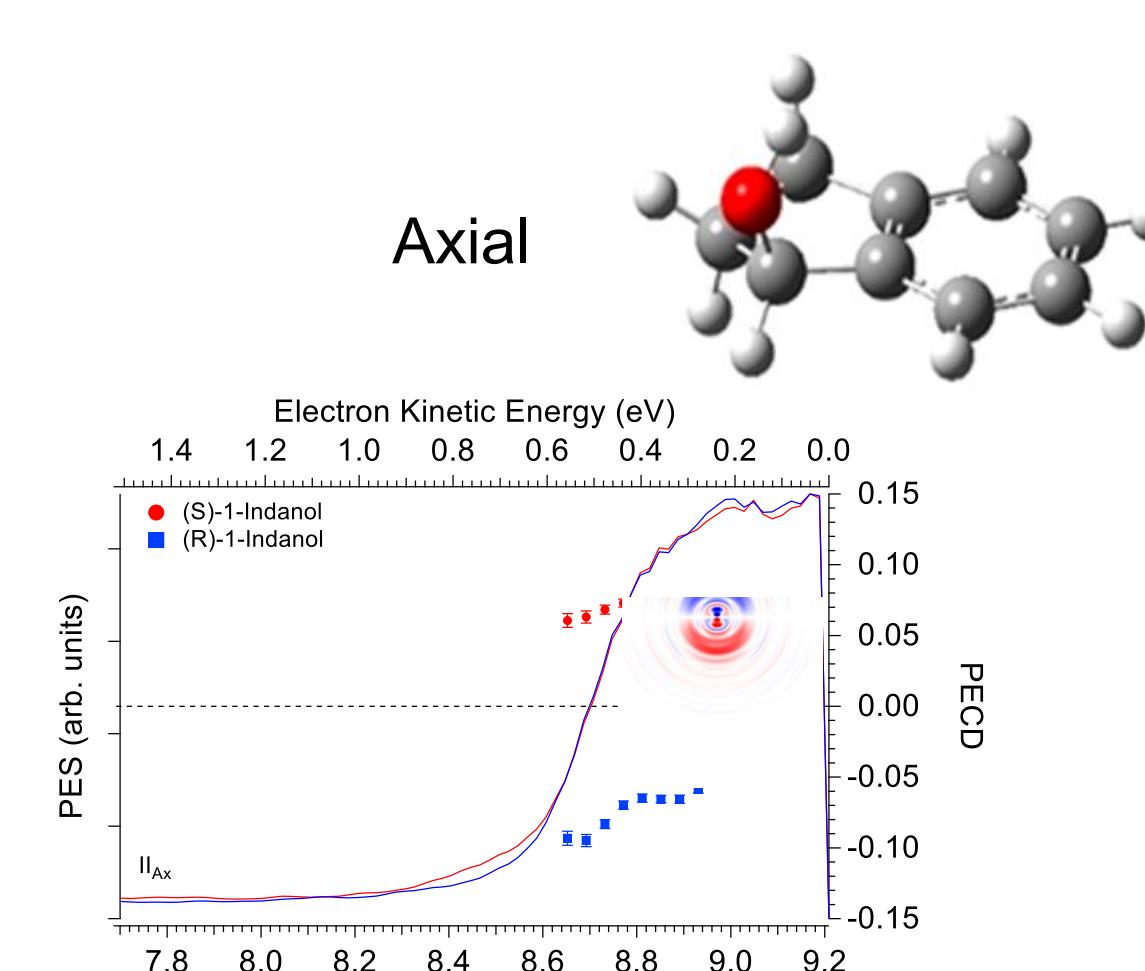
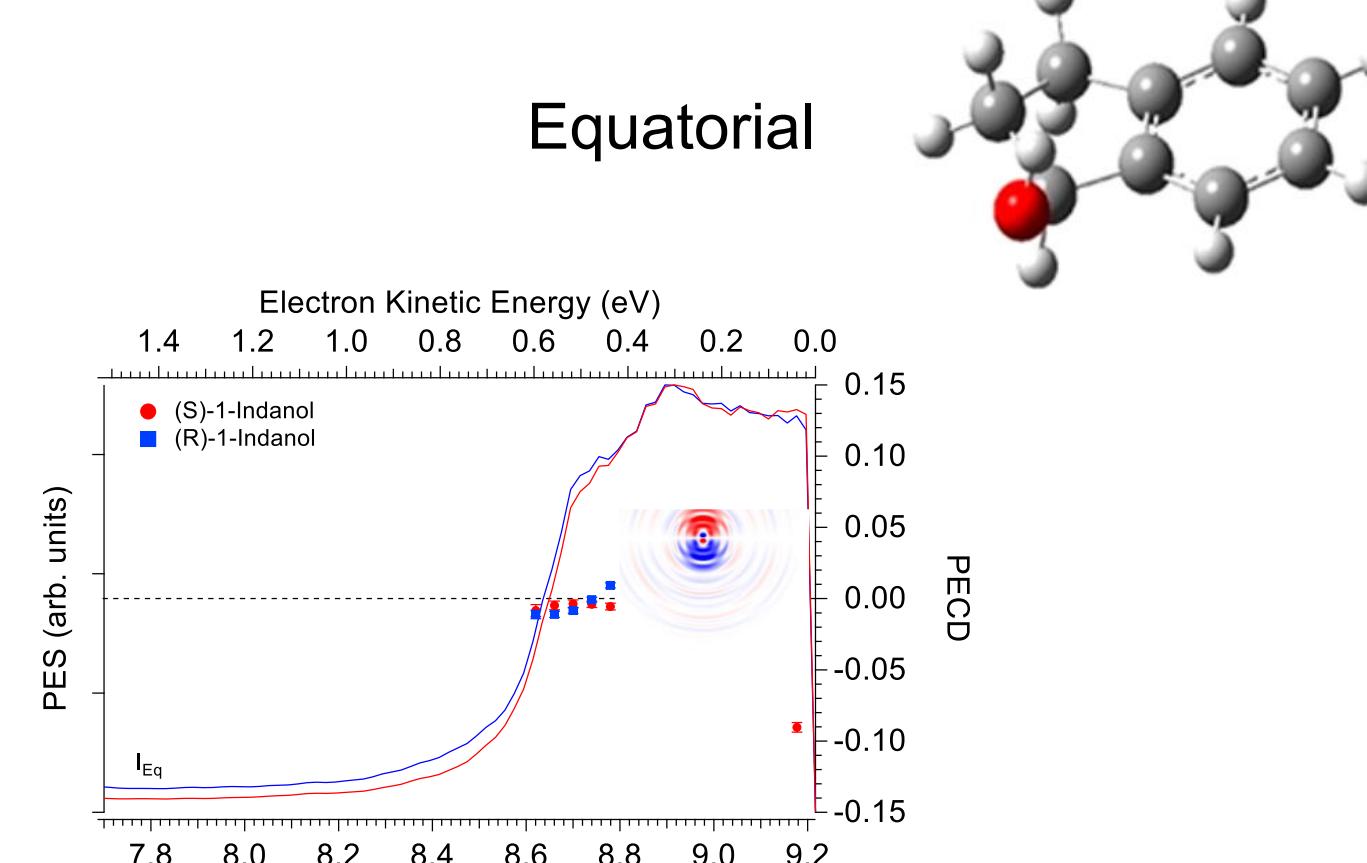


## Two-photon conformer specific PECD of 1-Indanol



$S_0$ - $S_1$  spectrum of 1-indanol in He. Transition origin 37073 cm<sup>-1</sup>

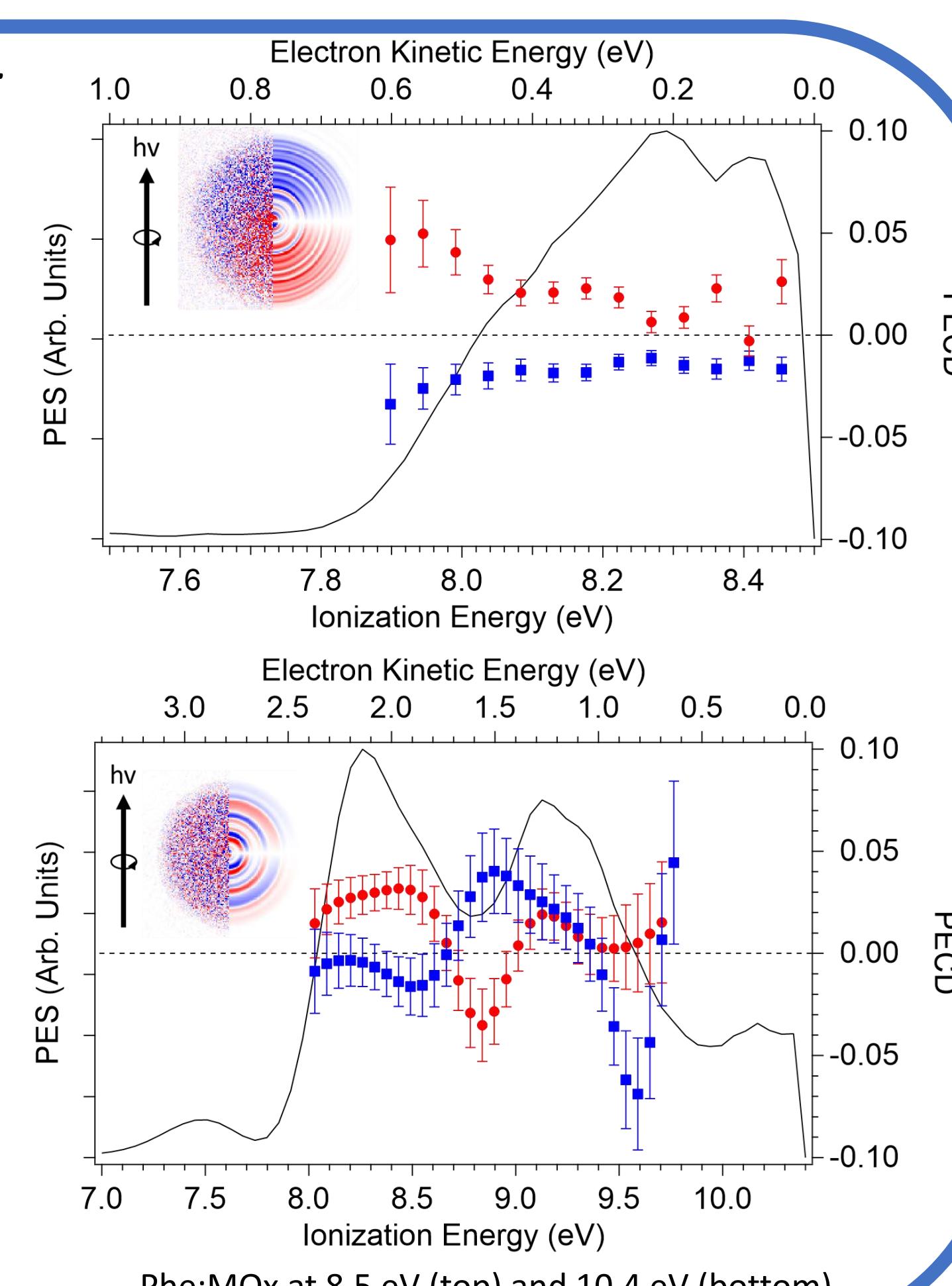
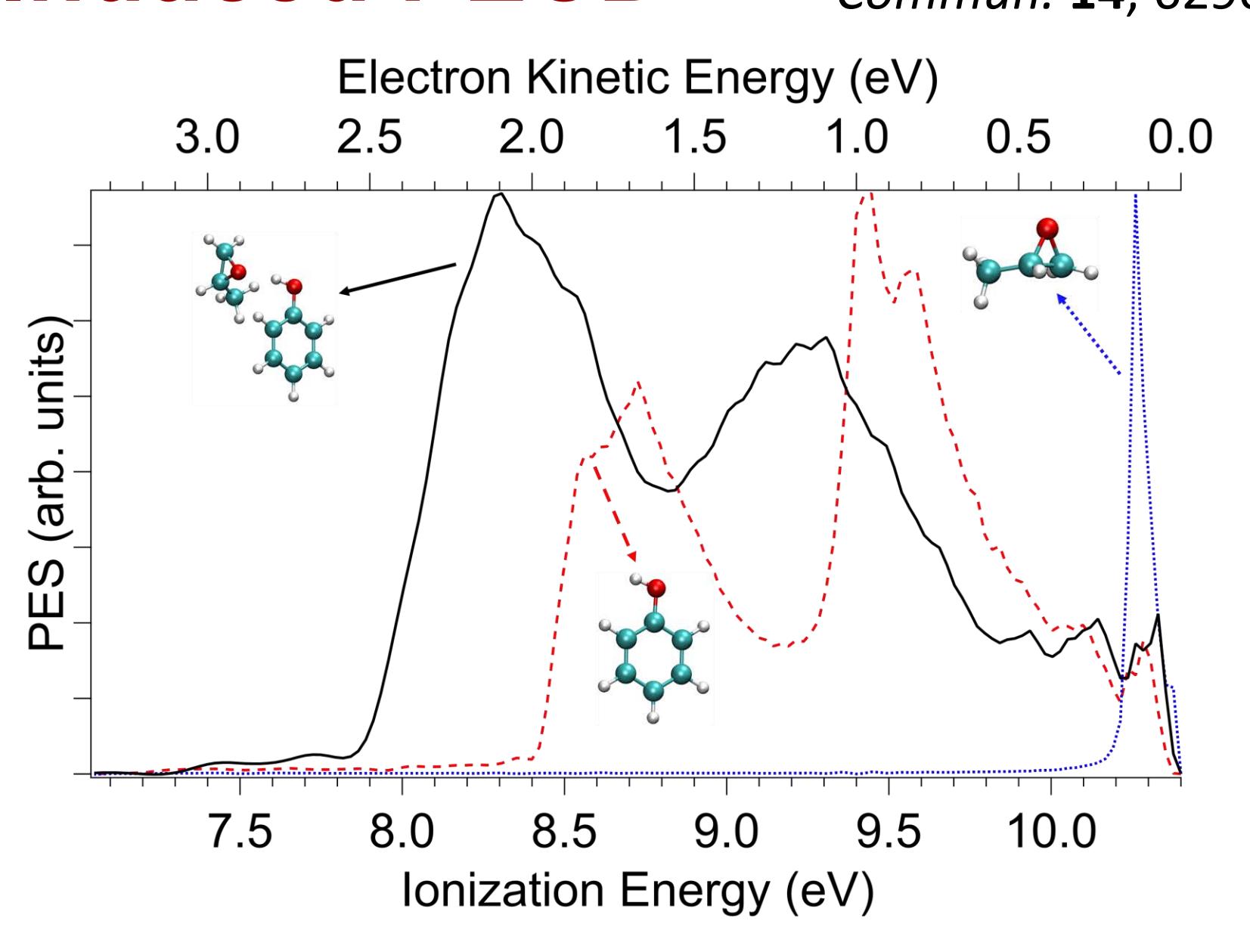
A. Bouchet et al. *Journal of Molecular Structure* (2014) **1076**, 344-351



**PECD and photoelectron spectra (PES) of 1-Indanol**  
Left: 0-0 origin transition of the equatorial conformer  
Right: 0-0 origin transition of the axial conformer

## Induced PECD

E. Rouquet et al., *Nat. Commun.* **14**, 6290 (2023)



## Conclusion

First ever true conformer specific PECD

- Use of a **ns-laser** + resonance enhanced two-photon ionization (**RE2PI**) → **conformer selection**
- PECD: particularly **sensitive to molecular structure and conformation**

First evidence of induced PECD

- **Analytical potential**, chiral recognition...

What's next ?

- **Two-color RE2PI** energy scheme
- **Time-resolved study** : see the **evolution** of induced PECD over dissociation of the complex (scale of the chiral interaction)
- Application of **two-photon PECD** on **molecular complexes** such as Phe:MOx

