



TREX WEBINAR

Quantum Package - User Feedback

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Laboratoire de Chimie Et Interdisciplinarité, Synthèse, Analyse, Modélisation



8th February 2023

Master 2 Internship, LCT, Sorbonne Université :

- With Emmanuel Giner and Julien Toulouse
- Multideterminant range separated DFT
- Development and implementation in QP

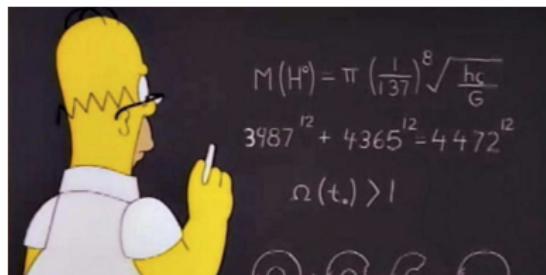
PhD, LCPMR, Sorbonne Université :

- With Stéphane Carniato and Richard Taïeb
- Description of double core hole spectroscopies
- Development and implementation in QP

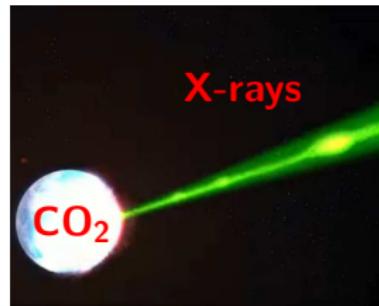
My PhD in a nutshell

Theoretical study of double ionisation/excitation in core shell

Quantum Chemistry



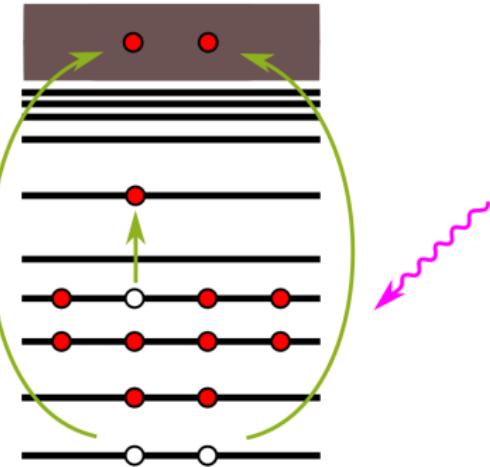
Computational Chemistry



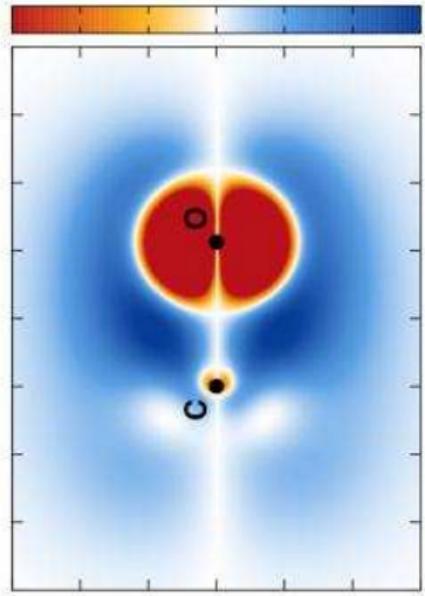
Spectroscopy - XPS

Why did we need new methodological developments ?

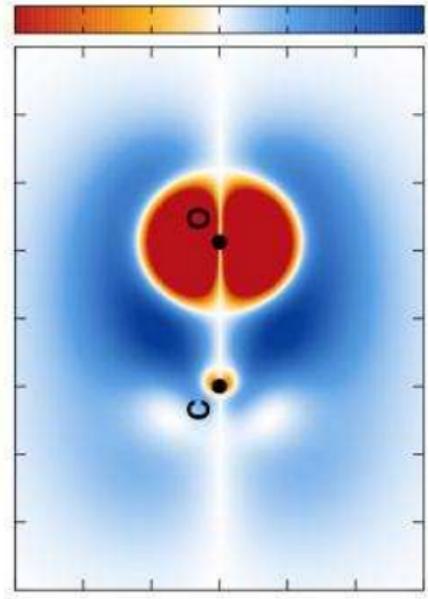
**Double
Photo-ionization**
+
Shake-up



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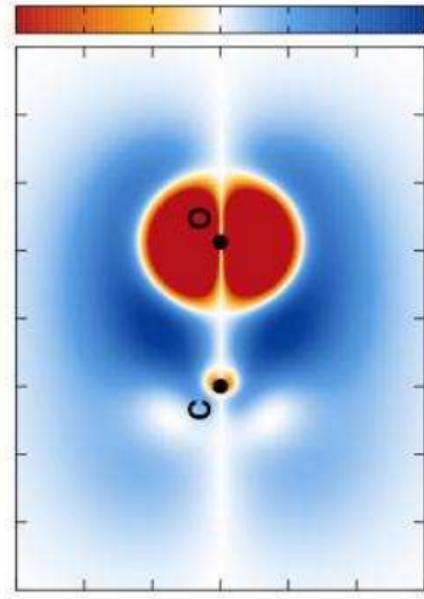
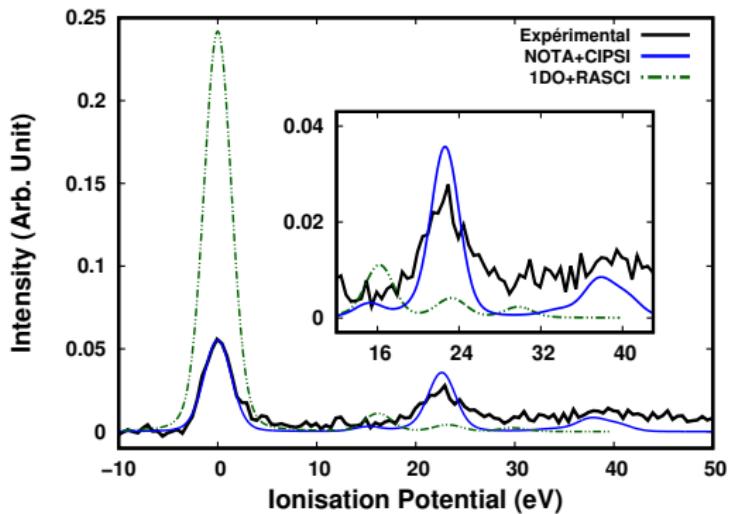


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- Easy to find pertinent documentation for developer
- Especially made to handle Slater determinants
- Produces high quality wave functions
- Helpful and Friendly team
- Free and Open source



What did I use Quantum Package for ?

Methodological aspects

Simulation / Production

Physics Interpretation

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Methodological aspects

- How to use the native programs of QP for core hole state calculation
- Development of a large plugin series fully interfaced with QP

Simulation / Production

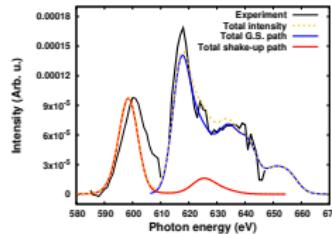
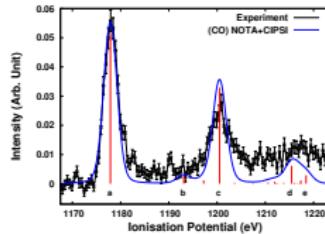
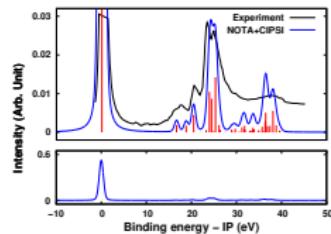
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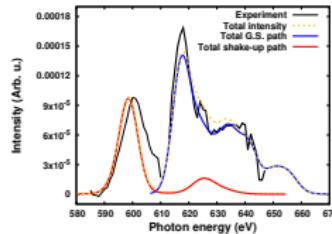
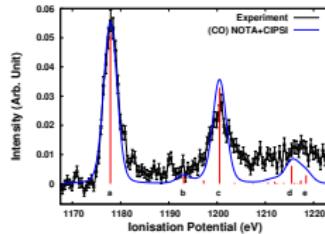
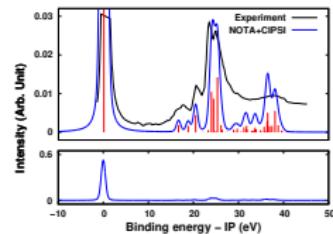
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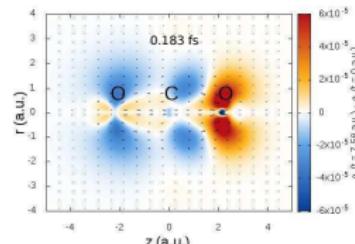
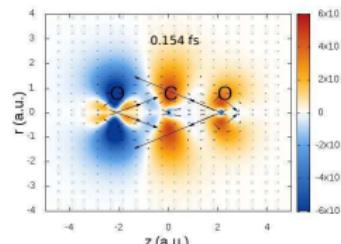
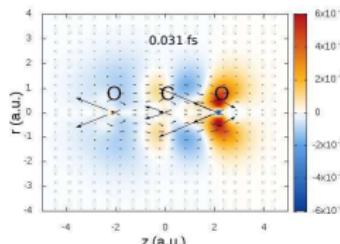
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Team ModES (CEISAM)

Experimentalist collaborators :
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Marc Simon *et al.*



Emmanuel Giner
Anthony Scemama



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