Chimie théorique des actinides

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Atelier PARIS 2011

Université Nice Sophia Antipolis, campus Valrose
8-9 Décembre 2011
Perspectives Scientifiques pour le GNR PARIS
Chimie des actinides

Remerciements :

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Publications 2011 dans le cadre de PARIS
Covalence dans des composés d'éléments f
Modélisations d'un actinide extrait en phase organique

Publications 2011 soutenues par PARIS

Inorganic Chemistry

ARTICLE

pubs.acs.org/IC

Inorg. Chem., 50 (10),(**2011**) 4572–4579. doi: 10.1021/ic200260r

Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution

Paola D'Angelo,*,† Andrea Zitolo,† Valentina Migliorati,† Giovanni Chillemi,‡ Magali Duvail,§ Pierre Vitorge,§,∥ Sacha Abadie,†,§ and Riccardo Spezia§

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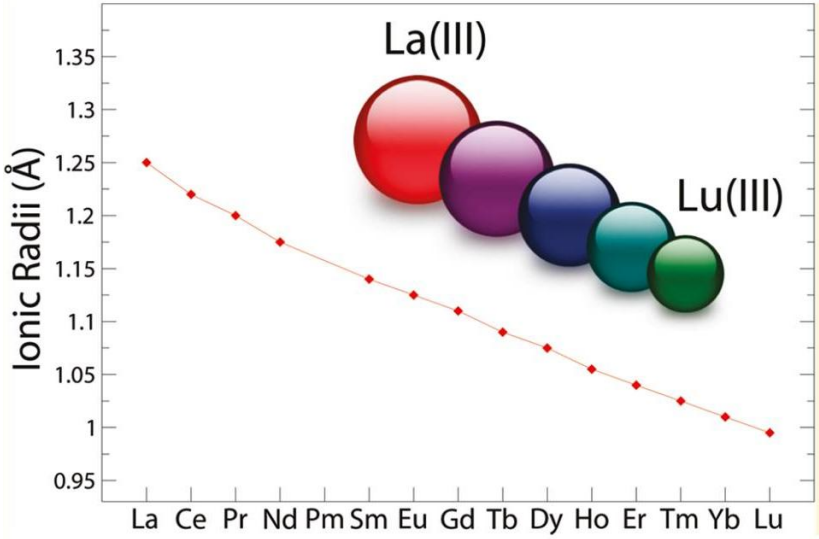

■ ACKNOWLEDGMENT

This work was supported by CASPUR with the Standard HPC Grant 2010 entitled "A combined X-ray absorption spectroscopy, Molecular Dynamics simulations and Quantum Mechanics calculation procedure for the structural characterization of ill-defined systems". We acknowledge the European Synchrotron Radiation Facility for provision of synchrotron radiation facilities and GNR-Paris for partial funding.

Publications 2011 soutenues par PARIS

AIP The Journal of Chemical Physics

Polarizable interaction potential for molecular dynamics simulations of actinoids(III) in liquid water

Magali Duvail, Fausto Martelli, Pierre Vitorge, and Riccardo Spezia

J.Chem.Phys. 135, (**2011**) 044503.
doi:10.1063/1.3613699

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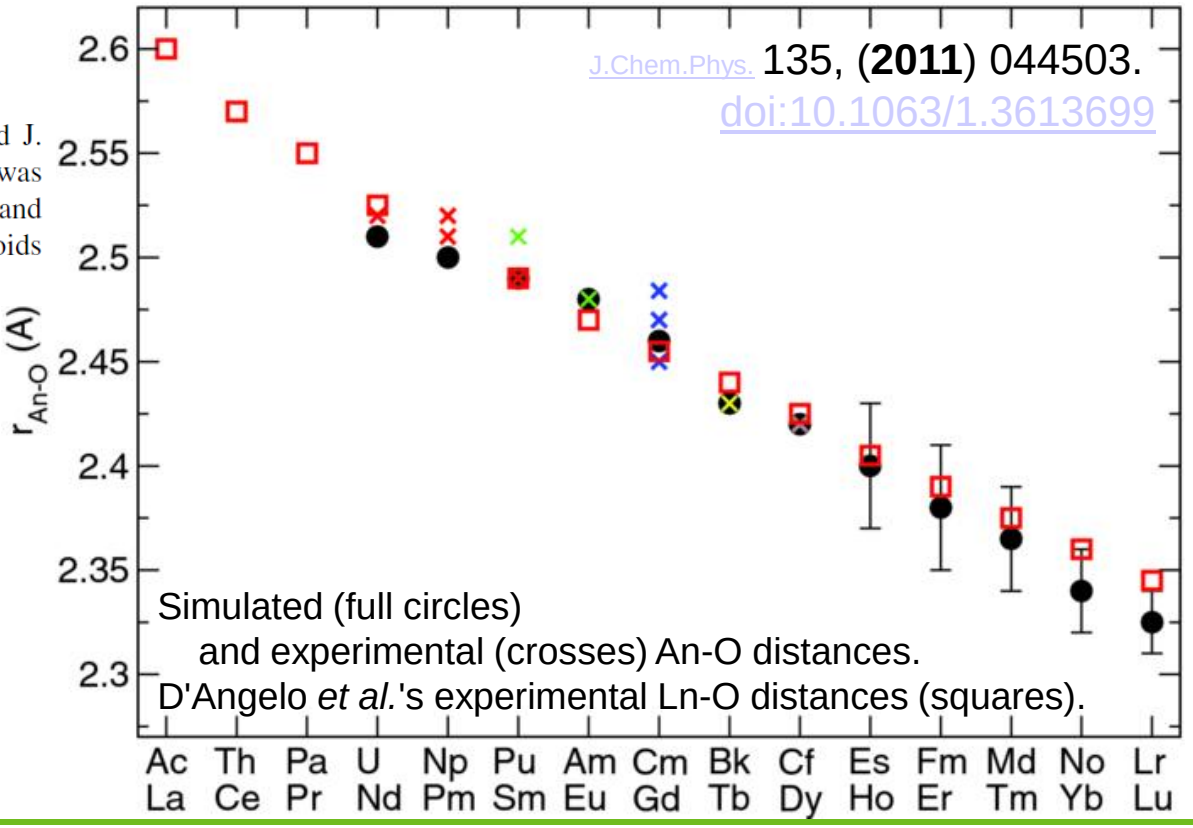

Simulated (full circles) and experimental (crosses) An-O distances.
D'Angelo *et al.*'s experimental Ln-O distances (squares).

Publications 2011 soutenues par PARIS

THE JOURNAL OF PHYSICAL CHEMISTRY B

ARTICLE

pubs.acs.org/JPCB

J. Phys. Chem. B (**2011**) 115 (13), pp 3560–3570. doi:10.1021/jp111726b

Stability and Instability of the Isoelectronic UO_2^{2+} and PaO_2^{+} Actinyl Oxo-Cations in Aqueous Solution from Density Functional Theory Based Molecular Dynamics

Riccardo Spezia,[*,†] Bertrand Siboulet,[‡] Sacha Abadie,[†,§] Rodolphe Vuilleumier,[§] and Pierre Vitorge[*,†,⊥]

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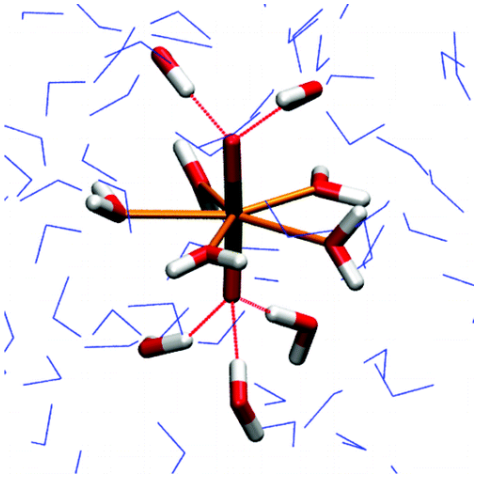

■ ACKNOWLEDGMENT

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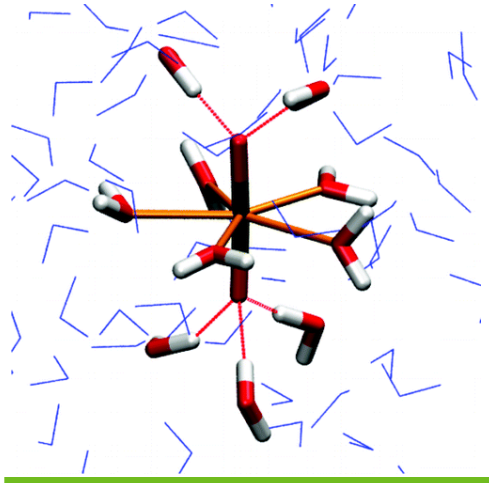
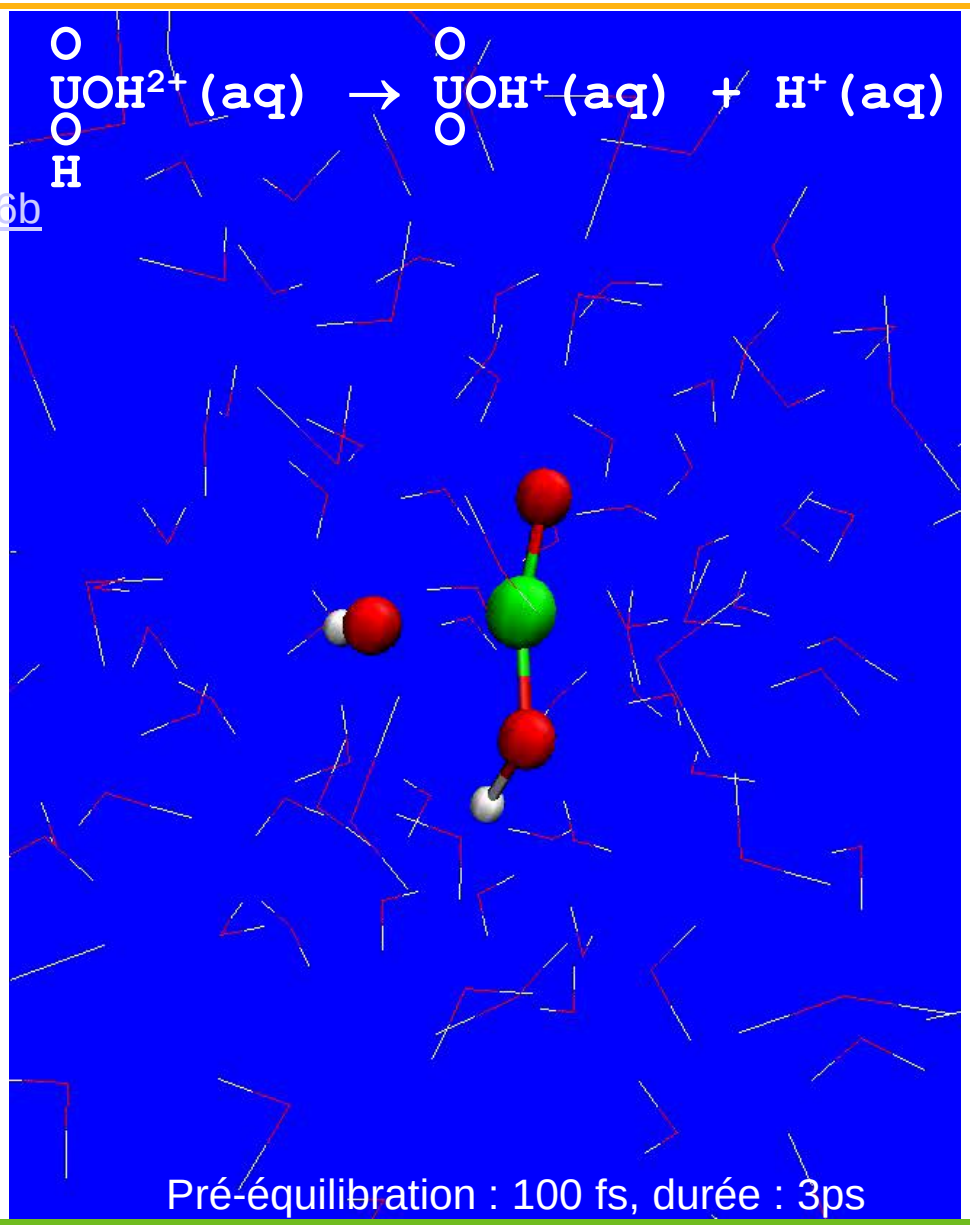
Simulation CPMD de $HOUO(OH)^{2+}(aq) \rightarrow OUO(OH)^{+}(aq) + H^{+}(aq)$

J. Phys. Chem. B (**2011**) 115 (13), pp 3560–3570. doi:10.1021/jp111726b

UMR8587 : Lambe

Riccardo Spezia,*,† Bertrand Siboulet, Sacha Abadie,†,§ Rodolphe Vuilleumier, and Pierre Vitorge



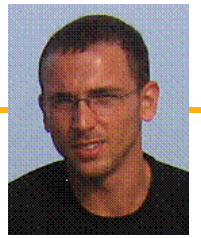


Pré-équilibration : 100 fs, durée : 3ps

Covalence dans des composés d'éléments f

Explication et prévision de la réactivité chimique en phase gazeuse, utilisée en spectrométrie de masse pour le dosage de combustible nucléaire irradié.

$$Ln^+ + NH_3 \rightarrow LnNH^+ + H_2$$

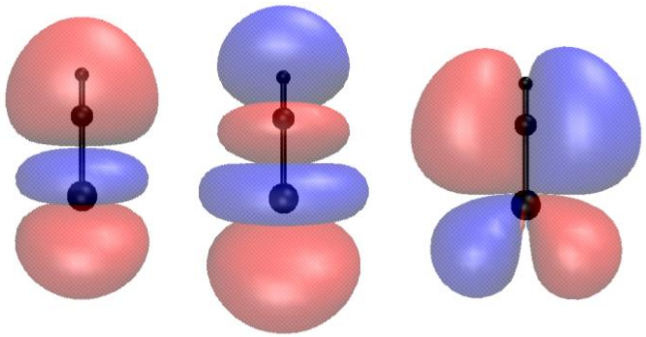


Alexandre Quemet, thèse en cours

UMR8587 : Lambe

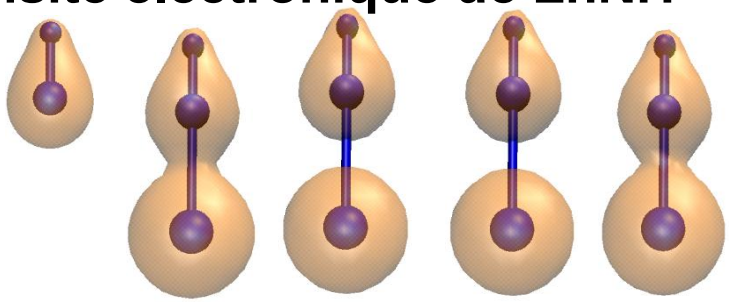
énergie atomique • énergies alternatives

La≡N-H$^+$



La	σ_{N-H}	σ_{La-N}	$(2)\pi_{La-N}$
La	6s 5p$_z$	6s 5p$_z$ 5d$_{z^2}$	5d$_{(x \text{ ou } y)z}$
N	2s 2p$_z$	2s 2p$_z$	2p$_{x \text{ ou } y}$
H	1s	1s	

Densité électronique de LnNH$^+$

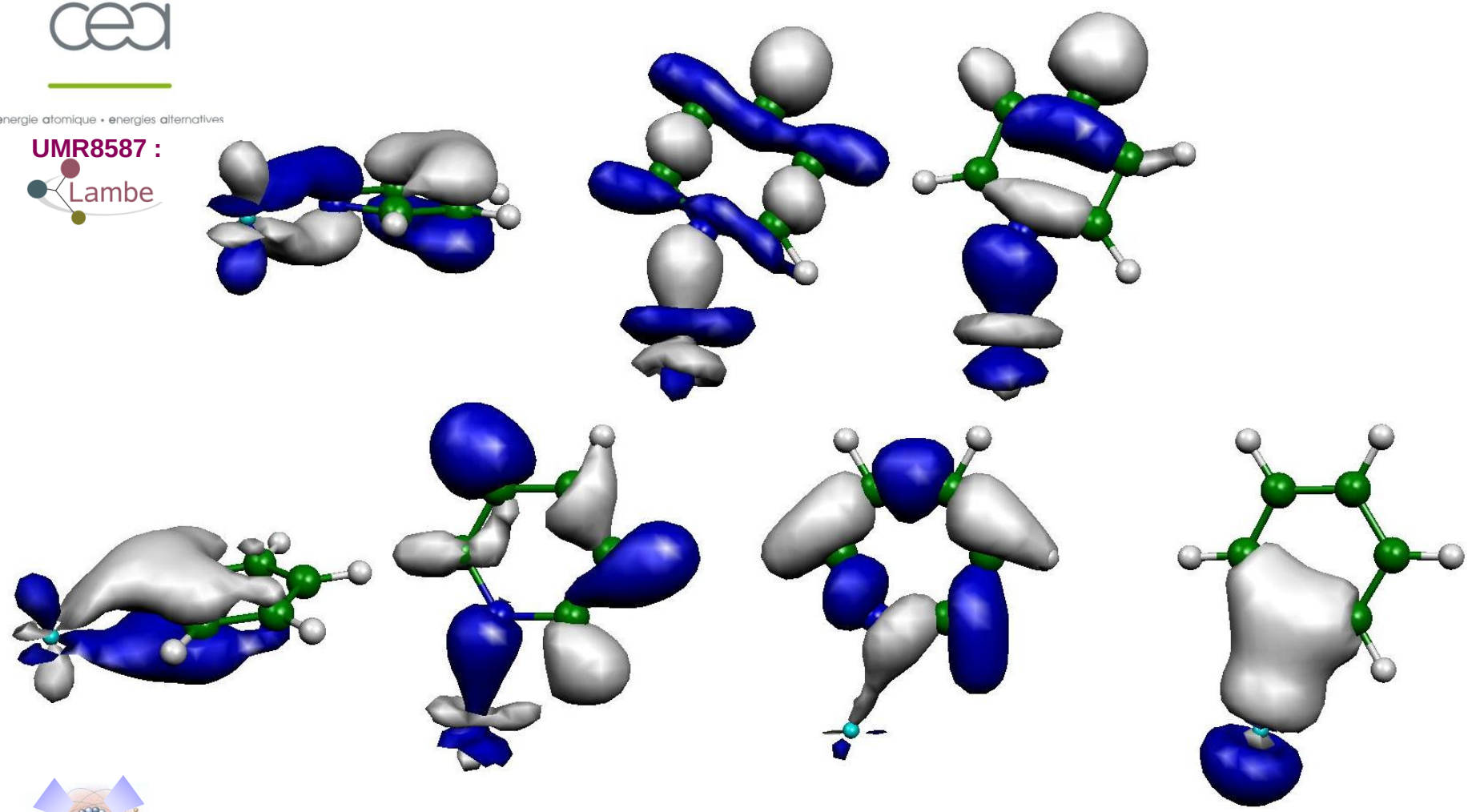


Ln La Sm Eu Gd

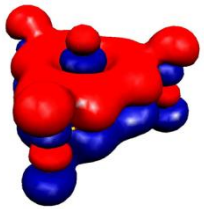
Covalence dans des composés d'éléments f

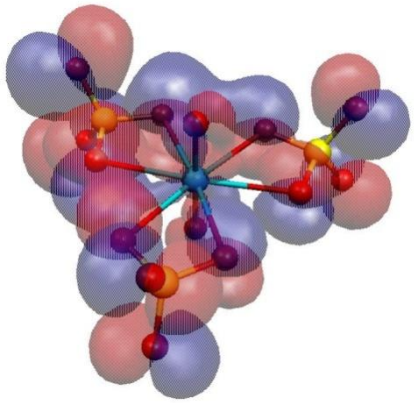
Liaison entre cation f et N (ou O) de ligands

(séparation des α...).

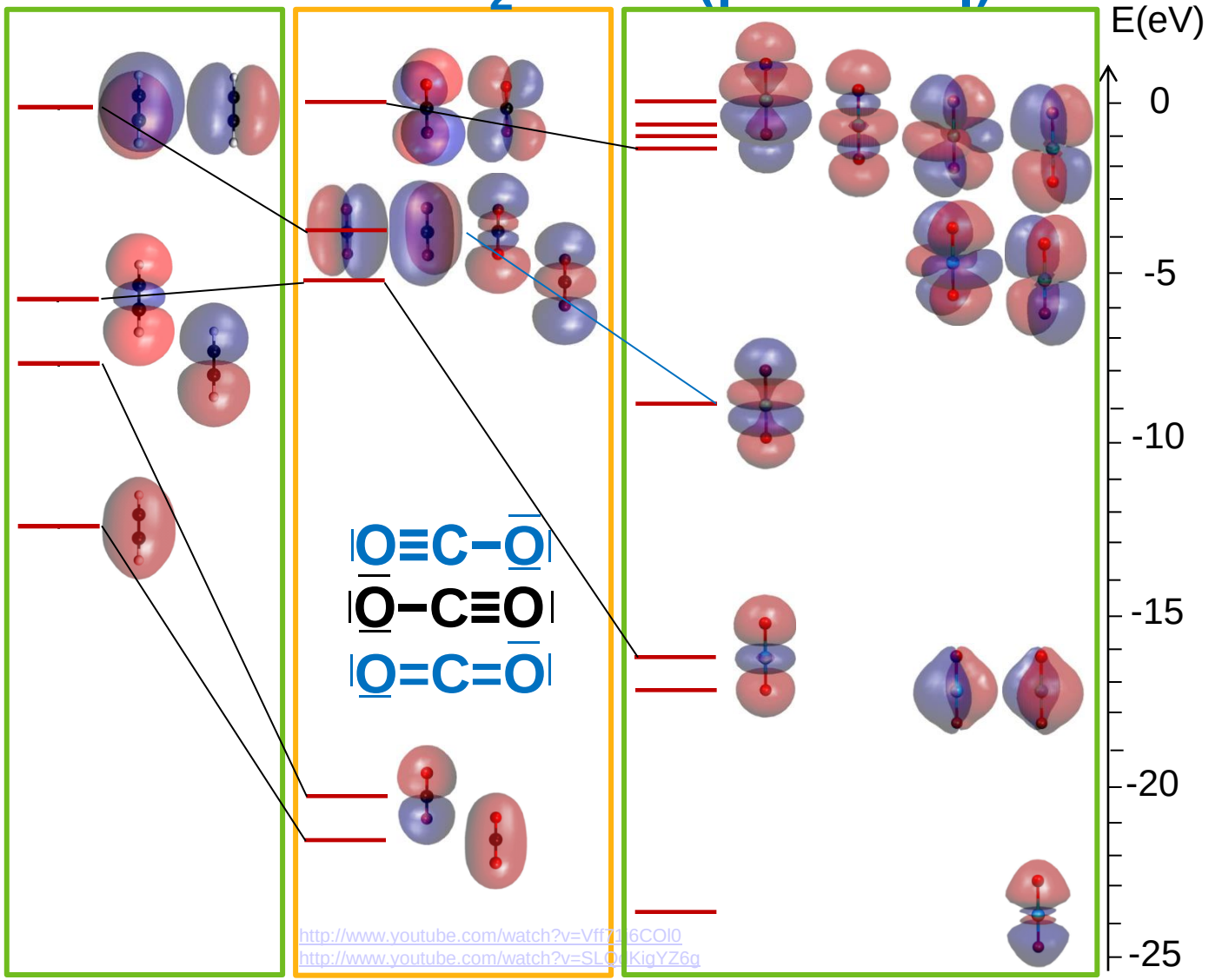


Covalence dans des composés d'éléments f



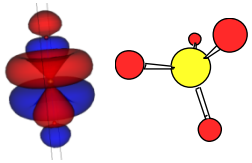


Abdelaziz Cadi-Essadek, stage ENSCBP



Modélisations d'un actinide extrait en phase organique

T.Ha Duong,
M.Masella,
D.Borgis,
J.-F.Dufrêche...



+ solvant explicite