Together with Professors Markus Meuwly in Lausanne, Qiang Cui in Boston, and a Dutch coordinator, Professor Celia Fonsecca-Guerra in Leiden, we propose to co-organize a Lorentz meeting which would focus on the modelling of Zn(II) and Ru(II) complexes.

Zn(II) is an essential co-factor of numerous Zn-metallo-enzymes, which play a prominent role in a diversity of cell growth and morphogenesis processes, but are responsible, when deregulated, for major diseases [L. Riccardi, V. Genna, M, De Vivo. 'Metal-Ligand Interactions in Drug Design'. *Nature Rev. Chem.,* **2018,** *2*, 100]. Although there are many high-resolution structures available, there still is nowadays a limited number of effective drugs [A. Y. Chen, R. N. Adamek, B. L. Dick, C. V. Credille, C. N. Morrison, S. M. Cohen. 'Targeting Metalloenzymes for Therapeutic Intervention'. *Chem. Rev*. **2019**, *119*, 1323].
We wish to bring together theoretical chemists, synthetic organic and inorganic chemists, biochemists and structural biologists. This could foster multi-disciplinary collaborations aiming at targeting some Zn-metallo-enzymes such as bacterial metallo-β-lactamases involved in the resistance of bacteria to antibiotics, histone deacetylase, histone decarboxylases, and matrix metalloproteinases. This would occur by a combination of diverse disciplines, including emerging accurate polarizable molecular dynamics potentials and semi-empirical DFT methods, structural biology, synthetic organic chemistry, and biochemistry.

There are emerging complexes of Ru(II) which could act as anti-cancer 'metallo-drugs' [Ang and Dyson, *Eur. J. Inorg. Chem.* **2006***,* 4003] and in photo-dynamics therapy [Mari et al., *Chem. Sci.* **2015,** *6,* 2660]. It would be very rewarding to bring together, in the context of a Lorentz meeting, quantum and computational chemists in the domains of time-dependent DFT and polarizable molecular dynamics, as well as photophysicists and organic chemists. This could enable to identify some privileged leads for the photosensitization of targets such as DNA and proteins such as kinases or superoxide dismutase.

This presentation is done in three parts. The first focuses on Zn(II) metalloproteins as targets for new drugs designed by joint experimental and computational approaches. The second focuses on Ru(II)-complexes as new-generation 'metallo-drugs' targeting DNA or proteins, and of potential chemotherapeutic interest. The third mentions the theoretical and experimental procedures resorted to. An organization schedule for the presentations is proposed at the end. The references given are from some of the contributors we intend to invite.

## 1. Zn(II) metalloproteins.

There are two essential Zn(II) metalloprotein targets: Zn-dependent metalloenzymes having a mono- or a binuclear Zn-catalytic site, and non-enzymatic Zn-proteins, such as retroviral Zn-fingers or steroid receptors.

***Zn-metalloenzymes****.* The following list is not limitative. We would like to mention:
a) Zn-metallo-β-lactamases (MBL), responsible for the acquired resistance of bacteria to antibiotics which they cleave and inactivate. There are two strains responsible for nosocomial diseases in hospitals: New Delhi MBL and VIM-2 (Verona Integrated MBL), against which there are no inhibitors of sufficient affinity and selectivity to be used as drugs. High-resolution X-ray structures are available [1, 2]. Therefore this would be an ideal topic for a collaboration associating: a) synthetic organic chemists, b) structural biologists, and theoretical chemists from both c) quantum chemistry and d) force-field development. A paper reporting on the results of a novel Zn-binding motive, triazole thione (TZT), and its complexes with the binuclear Zn-binding sites of L1 and Vim2 strains was recently published by one of us, jointly with experimentalists [3], and efforts are underway on a series of TZT-containing VIM2 inhibitors. Promising new leads, which

could also lend themselves to joint experimental and computational studies, are in the class of boron-based compounds [4].
b) histone deacetylase (HDAC), a class of enzymes removing acetyl groups from an N-acetyl lysine amino acid on a histone, allowing the histones to wrap the DNA more tightly. Upregulated HDAC activity is observed in cancer and neurodegenerative disease. HDACs are among the most promising therapeutic targets for anti-cancer inhibitor design [5, 6].
c) histone demethylases, which remove a terminal methyl group from Lys or Arg residues in histones. As for HDAC. their overexpression is linked to cancer [7].
d) Zn-dependent metalloproteinases, which belong to several classes, denoted as MMP-1 to MMP-12. They are responsible for metastases, tumor cell invasion, auto-immune diseases, neuro-inflammation, arthritis. There are several high-resolution X-ray structures, but few, if at all, efficient inhibitors [8, 9].
e) Phosphomannose isomerase (PMI), responsible for microbial and parasitic diseases [10].

***Non-enzymatic Zn-fingers.***
***Retroviral proteins.*** A prominent example is the the nucleocapsid of HIV-1 retrovirus, denoted as NCp7, which has two invariant Zn-fingers. These play an essential role in the chaperone activity of NCp7 on DNA [11]. Contrary to the HIV-1 protease, reverse transcriptase and integrase, NCp7 cannot evade treatment by mutations as these inactivate the virus. NCp7 is thus a target for anti-retroviral therapies [12, 13]. The Laboratoire de Chimie Theorique has an earlier contribution with the National Institute of Health in Bethesda [14], which we plan to reactivate, and an ongoing one with the Laboratoire de Pharmacologie Structurale in Paris [15] aiming at the design of novel inhibitors targeting a complex between NCp7 and DNA [11].
***Steroid receptors***. Steroid or nuclear hormone receptors constitute an important superfamily of transcription regulators [16]. Their DNA-binding domains consist of two zinc-nucleated modules and a C-terminal extension. Residues in the first zinc module determine the specificity of the DNA recognition and residues in the second zinc module are involved in dimerisation. They are involved in diverse functions, including control of embryonic development, cell differentiation and homeostasis. When overexpressed, they lead to disease, and are thus also a target for drug design.

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15. Reconciling NMR Structures of the HIV-1 Nucleocapsid Protein (NCp7) using Extensive Polarizable Force Field Free-Energy Simulations. L. El Khoury, F. Célerse, Louis Lagardère, L.-.H Jolly, E. Derat, Z. Hobaika, R. G. Maroun, P. Ren, S. Bouaziz, N. Gresh, J.-P. Piquemal, 2020, submitted (11/19)[HAL][ChemRxiv]. DOI: 10.26434/chemrxiv.11336975.v
16. Common architecture of nuclear receptor heterodimers on DNA direct repeat elements with different spacings. N. Rochel, F. Ciesielski, J. Godet, E. Moman, M. Roessle, C. Peluso-Iltis, M. Moulin, M. Haertlein, P. Callow, Y. Mély, D. I Svergun, D.Moras. *Nature Structural Molecular Biology* **2011***, 18,* 564.

## 2. Ru(II)-based metallodrugs.

Ru(II)-coordination complexes are an emerging class of 'metallo-drugs' [1] which can bind to protein targets such as kinases [2], as well as to DNA [3]. A notable difference with respect to the other major class of metallodrugs, namely Pt(II) complexes, is their photoactivable character under infra-red radiation. They could be used in non-invasive photodynamic therapy against cancer, owing to the longer penetration of IR radiation in the body. Several potential Ru(II) metallodrugs have been put forth, such as ruthenium arene, Ru(II)-polypyridyl complexes, and some complexes with DNA or a kinase protein have been characterized [4-7]. Complexes of Ru(II) with nucleobases have lent themselves to QC studies [8]. It could be very rewarding to design derivatives with enhanced affinities and selectivity for their DNA or protein targets. This could be enabled by a synergistic use of polarizable molecular dynamics and the so-called 'QM/PMM' approach [9]. In this context, a core surrounding Ru(II) could be treated quantum mechanically, and the rest of the protein or DNA target, by classical polarizable molecular mechanics. The latter approach could be essential to study the photoactivation process under the effect of IR radiation, resorting to time-dependent DFT. The structures then used would be the lowest-energy poses resulting from polarizable molecular dynamics.
The design of Ru(II)-based supramolecular complexes with photoactivable properties constitutes another important topic for joint experimental and theoretical approaches [10].

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*ChemBioChem* **2019,** *20,* 1.
8. Interactions of the "piano□stool" [ruthenium(II) (η6□arene)(en)CL]+ complexes with water and nucleobases; ab initio and DFT study. Z,Futera, J. Klenko, J E. Šponer, J. Šponer, J. V. Burda. *J Comput. Chem*. **2009**, *30*, 1758.
9. Towards Large Scale Hybrid QM/MM Dynamics of Complex Systems with Advanced Point Dipole Polarizable Embeddings. D. Loco, L. Lagardere, G. A. Cisneros, G. Scalmani, M. Frisch, F.Lipparini, B. Mennucci, J.-P. Piquemal. *Chem. Sci.* **2019,** *10,* 7200.
10. Supramolecular Cages Incorporating Photoactive Noble Metal Complexes. D. R. Martir, E. Zysman-Colman. *Chem. Commun.* **2019**, *55*, 139.

## 3. Computational procedures.

The main two procedures will be quantum chemistry: ab initio (QC), DFT and tight-binding DFT (DFT-TB), and polarizable molecular mechanics/dynamics (PMM/PMD). All four coorganizers have contributions in either field with applications to biological molecules [1-4].
QC is used to calibrate and validate PMM/PMD and to enable QM/MM studies. Regarding Zn-metalloenzymes, the latter approach could be used to simulate the mechanism of enzymatic cleavage. Regarding Ru(II) metallodrugs, they could be used to simulate the mechanism of light activation on radical-induced cleavage of the DNA or protein targets.
PMD is benefiting from dramatic enhancements of the computational speed. These have resulted from massive parallelism, considerable speed-ups in the computation of the iterative polarization, and more efficient integrators. It should now be possible to use PMD in long-duration MD, enabling a more detailed exploration of the potential energy hypersurface of the ligand-macromolecule complexes.

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2. A. S. Christensen, T. Kubar, Q. Cui, M. Elstner. Semi-empirical Quantum Mechanical Methods for Non-covalent Interactions for Chemical and Biochemical Applications, *Chem. Rev.* **2016**, *116*, 5301.

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4. Complexes of a Zn-Metalloenzyme Binding Site with Hydroxamate-Containing Ligands. A Case for Detailed Benchmarkings of Polarizable Molecular Mechanics/ Dynamics Potentials When the Experimental Binding Structure is Unknown.. N. Gresh, D. Perahia, B. de Courcy, J. Foret, C. Roux, L. El-Khoury, J.-P. Piquemal, L. Salmon, *J. Comput. Chem.,* **2016**, *37*, 2770.

**Organization**.

The five-day conference could be organized as follows.

*First day.* Morning session. Presentation by experimentalists of Zn-metalloenzymes (I).
Afternoon session. Presentation by experimentalists of Ru(II) metallodrugs (I).

*Second day.* Morning session. Presentations of advances in PMM/PMD (I).
Afternoon session. Presentation by experimentalists of Zn-metalloenzymes (II).
Some 'flash' presentations.

*Third day.* Morning session. Presentations of advances in QC, DFT, and DFT-TB (I).
Afternoon session. Presentation by experimentalists of Ru(II) metallodrugs (II).
Some 'flash' presentations.

*Fourth day.* Morning. Presentation by experimentalists of non-enzymatic Zn-metalloproteins.
Afternoon. Presentation of advances in QC, DFT, DFT-TB, and PMM/PMD (I).
Discussion in one or two groups.

*Fifth day.* Morning. Presentation of advances in PMM/PMD, and QC, DFT, and DFT-TB (II).
Afternoon. Discussion in one or two groups.

**Requested fundings from CECAM-FR-MOSER: 3000 euros**

List of proposed participants.

1. Zn-metalloproteins.

Zn-metalloenzymes.

1. Christopher Schofield. Oxford University
http://schofield.chem.ox.ac.uk/antibiotics.aspx
MBL targeting

2. David W. Christianson. University of Pennsylvania
https://live-sas-www-chem.pantheon.sas.upenn.edu/profile/david-w-christianson.
Histone Deacetylase Structure and Function

3. Seth Cohen. University of California at San Diego
http://cohenlab.ucsd.edu
Design, synthesis, and evaluation of inhibitors of metalloproteins.

4. Marco De Vivo. Laboratory of Molecular Modeling and Drug Discovery, Istituto Italiano di Tecnologia, Genoa, Italy.
Ligand-metal interactions in biomolecules.

5. Jean-Francois Hernandez. Laboratoire des Biomolecules Max Mousseron, Universite de Montpellier.
Ibmmpeptide.com/jean-francois-hernandez
Design and synthesis of MBL inhibitors

6. Vincent Dive, Centre d'Etudes Atomiques, Saclay
http://joliot.cea.fr/drf/joliot/Pages/Entites_de_recherche/medicaments_technologies_sante/SIMOPRO/lcv.aspx
Zn-metalloprotease inhibition.

7-8. Maria Ramos, Sergio Sousa, University of Porto
https://www.fc.up.pt/pessoas/mjramos/index.html
https://biosim.pt/sergio-f-sousa/
Zn metallo-proteinase inhibition.

9. Laurent Salmon, University of Paris-Saclay
https://www.icmmo.u-psud.fr/fr/perso/laurent-salmon
Design, synthesis and tests of Zn-dependent metalloenzymes
10. Bogdan Iorga, Institut de Chimie des Substances Naturelles, Gif-sur-Yvette,
Design of inhibitors of Zn-MBL.
11. Lars Hemmingsen. University of Copenhagen
https://chem.ku.dk/ansatte/alle/?pure=en/persons/124560
Design of MBL inhibitors
12. Lars Olsen. Department of Drug Design and Pharmacology, University of Copenhagen
https://www.researchgate.net/profile/Lars_Olsen5.
Histone demethylase targeting.
13. Natalie Strynadka. University of British Columbia, Vancouver
http://strynadkalab.biochem.ubc.ca/research/antibiotic-resistance.php
X-ray structure of New-Delhi MBL.

14. Jean-Denis Docquier University of Sienna, Italy.
https://www.researchgate.net/profile/Jean_Denis_Docquier
X-ray structure of VIM-2 MBL.

Non-enzymatic Zn-metalloproteins.

15, 16. Ettore Appella, Lisa Miller Jenkins
National Institute of Health, Bethesda, Maryland.
https://irp.nih.gov/pi/ettore-appella

17. Yves Mely
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http://www-lbp.unistra.fr/rubrique33.html?lang=fr

18. Serge Bouaziz
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2. Ru(II)-based compounds.

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http://www.gassergroup.com/gilles-gasser.
Ru(II)-based photoactivating compounds.

20, 21. Antonio Monari, Xavier L. Assfeld. Laboratoire de Physico-Chimie Theorique, Nancy.https://lpct.univ-lorraine.fr/
Complexes of Ru(II) metallodrugs with DNA.
22. Sylvestre Bonnet. University of Leiden, Leiden institute of Chemistry.
https://www.universiteitleiden.nl › staffmembers › sylvestre-bonnet
Light activation of Ru(II) metallodrug complexes with oligonucleotides.
23. Eric Meggers, University of Marburg. https://www.uni-marburg.de/fb15/ag-meggers?language_sync=1
Design of metallo-drugs.

24. Nils Metzler Nolte, University of Bochum.
https://www.ruhr-uni-bochum.de/zemos/nolte
Design of metallo-drugs.

25. Paul Dyson, Ecole Polytechnique Federale de Lausanne.
https://www.epfl.ch/labs/lcom/dyson/.
Design of anti-cancer Ru(II) metallodrugs.

26. Christian Hartinger. University of New Zealand in Auckland
https://unidirectory.auckland.ac.nz/profile/c-hartinger.
Ru(II)-based metallo-drugs.

27. Jacqueline K. Barton. California Institute of Technology, Pasadena.
http://Cce.caltech.edu/people/Jacqueline-k-barton.

Synthesis and characterization of DNA-binding probes.

28. Eli Zysman-Colman, University of St Andrews
http://www.zysman-colman.com/research_en.php
Design of supra-molecular materials

3. Theoretical and computational chemistry.

29. Dennis R. Salahub, University of Calgary
https://www.ucalgary.ca/dennis-salahub-lab/profiles/dennis-salahub.

30. Ursula Rothlisberger, Ecole Polytechnique Federale de Lausanne
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31. Kenneth K. Merz, Michigan State University
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36. Pengyu Ren, University of Texas at Austin
https://cns.utexas.edu/directory/item/1577-ren-pengyu?Itemid=349

37. Michael Schnieders, University of Iowa
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38. Clotilde Policar, Ecole Normale Superieure, Paris.
https://www.chimie.ens.fr/recherche/laboratoire-lbm/peptides-glycoconjugues-metaux-biologie/people/clotilde-policar/

39. Celia Fonsecca-Guerra University of Leiden
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41. Markus Meuwly, University of Basel
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42. Nohad Gresh, Laboratoire de Chimie Theorique, Paris.
https://scholar.google.fr/citations?user=V4pAy7YAAAAJ&hl=fr

Bruno Chaudret.

http://lpcno.insa-toulouse.fr/spip.php?page=biblio&qui=676&lang=en
Design of Ru(II)-based nanoparticles.

Organometallic Ruthenium Nanoparticles : Synthesis, Surface Chemistry, and Insights into Ligand Coordination
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Cusinato, Lucy ; Martinez-Prieto, Luis M. ; Chaudret, Bruno ; del Rosal, Iker ; Poteau, Romuald
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