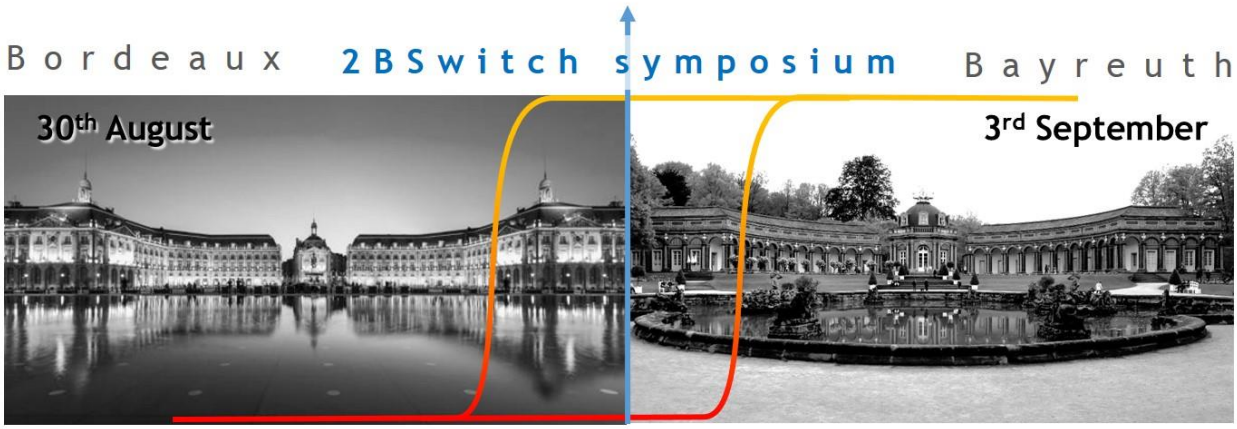

2021 is still under the influence of Covid-19, affecting many events and forcing every researcher to rethink its way of sharing science. This year again, the international community working on spin state switching is gathered in a virtual event. The Bordeaux-Bayreuth symposium on spin state switching, 2B-Switch, is an online meeting co-organized by Birgit Weber and Guillaume Chastanet to keep the link within the growing "switching" community members. This wouldn't have been possible without the kindness of all the invited speakers who accepted to take on this adventure with us. We want to thank them all for their support, patience and investment.

This 2B-Switch event gathers 26 oral presentations and 33 posters (including 18 flash presentations) from USA, Japan, Thailand, New-Zealand, France, Spain, Ireland, UK, Germany, Canada, Romania, Australia, Switzerland, India, Greece, Czech Republic, China (in no particular order). The program has been set up to account for the time shift between all these countries, which was an almost impossible task with 16 hours of difference between our two most chronologically distant speakers. We tried to find the tools to overcome some of these difficulties and to keep discussions at the core of this event. We hope you'll enjoy this 2B-Switch symposium.

Let's discuss.

Birgit & Guillaume

websites: http://www.book-d.cnrs.fr/ or https://www.ac4.uni-bayreuth.de/de/2BSwitch-2021/index.html.

PROGRAM

August 30th	August 31th	September 1st	September 2d
	9h00-10h30 : Tong Bosckovic **6 flash talks**	9h00-10h30 : Ohba Tao Tuczek	9h00-10h30 : Brooker Takahashi Kurz
	10h30-11h00 : break	10h30-11h00 : break	10h30-11h00 : break
	11h00-12h30 : Bao Harding Real	11h00-12h30 : Tangoulis Triki Romero	11h00-12h30 : Marchivie Mondal Aromi
14h00-16h00 : Collet Shepherd Routaboul **6 flash talks**	14h00-16h00 : Frank Singh Fedin Krüger		
16h00-16h30 : break			
16h30-18h00 : Shatruk Morgan **6 flash talks**			

All presentations will be performed using Zoom. Every half-day will have its own link and password that will be sent to the registered participants. During the breaks we will provide breakout rooms for discussions in smaller groups. You are welcome to try them out!

- The concept of this meeting is to leave plenty of time for **discussion**.
- **Oral presentations** will last 20 minutes followed by at least 10 minutes of discussion moderated by the chair of the session.
- **The flash presentations** should last 5 mins, without Q&A session.
- **The posters** will be available all along the week to allow everybody to look at them and interact with the presenters through a dedicated chat.

1. Oral presentations

The oral presentations will be performed live. The talks should last 20 mn, followed by 10 mn of discussion.

In order that participants from all the countries and continents can see all the presentations, we would like to store them on a dedicated and protected site, only visible (not to download) for an additional week. Therefore, we ask the speakers if they allow us to record the presentation. We will promote discussions, giving access to the microphone and video to participants who would have indicated their will to ask question or to comment.

2. Poster presentations

A dedicated website will be used for the poster session. Each poster will have a space for 4 slides and a related chat. Students are invited to present a poster, composed of 4 slides in landscape format, with sufficient high resolution and size (font, figures,…) that it may be visualized easily in a standard 17 to 20” screen.

The corresponding files in pdf or ppt format must be sent to us by **Tuesday 24th of August**. We will upload them on the dedicated website and give you access through a password. An audio

file presenting briefly (4 mins maximum, saying on which slide you are talking) the poster can accompany the uploaded too.

They will be accessible all along the 2BSwitch event and one week after, remaining open for discussions.

Ethical considerations.

To promote discussions and exchanges around new results in a trustful atmosphere, and as part of the open science policy from the European community, this event is under the European charter for researchers. The results presented during this conference must not be used or diffused (in other conferences or articles, on social media…) without the agreement of the authors.

By registering and participating to this event, you agree with these ethical considerations.

DETAILED PROGRAM

All the Zoom sessions will be opened 30 mns before to let everyone come in and check everything is working.

Monday, 30th of August:

14h-16h, zoom session: to be defined

- *Introduction*
- Eric Collet: *Spin crossover, charge transfer and symmetry breaking: unsymmetric hysteresis loop and sequence of phases*
- Helena Shepherd: *A Supramolecular Approach to Controlling Spin Crossover Properties*
- Lucie Routaboul: *Post-synthetic modification of iron-triazole SCO complexes*
- *Flash talks*
    - P 01, Zackery C. Watts**:** *Exploring the spin-crossover and conductive nature of heteroleptic Fe/Co complexes with redox-active phenalenol-substituted ligands*
    - P 02, Thilini K. Ekanayaka*: Influence of the magnetic field on the thermal activation barrier of spin-crossover materials*
    - P 03, Krishna Kaushik**:** *Reversible Photo and Thermo-induced Spin-State Switching in a heterometallic {5d-3d} W_2Fe_2 Molecular Square Complex*
    - P 04, SandugashYergeshbayeva**:** *Spin-crossover in iron (II) complexes with π-extended 2,2'-biimidazole ligands*
    - P 05, Alexandra-Ioana Popa**:** *Isotropic and anisotropic behavior in spin crossover molecular magnets through the mechanoelastic model*
    - P 06, Patroula Gkolfi**:** *A facile approach to prepare silica hybrid, spin crossover water-soluble nanoparticles as a potential platform for thermally responsive MRI agents*

16h30-18h, zoom session: to be defined

- Michael Shatruk: *Design of sublimable and exfoliable spin-crossover materials*
- Grace Morgan: *Domain Wall Dynamics in Ferroelastic Spin Crossover Complexes*
- *Flash talks*
    - P 07, Maria Teresa Delgado Perez **:** *3D spin crossover nanocrystals with operative bistable switching properties*
    - P 08, Margaux Pénicaud**:** *Investigation of an Fe(II) SCO complex based on a heteroscorpionate ligand*
    - P 09, Irene Sanchez-Molina**:** *Modulation of the fluorescence of polyfluorene with spin-crossover*
    - P 10, Ramon Torres-Cavanillas**:** *Smart molecular/MoS_2 heterostructures featuring light and thermally-induced strain driven by spin switching*
    - P 11, Giada Truccolo**:** *Investigation of the role of modulators in the synthesis of new Hofmann-type MOFs*
    - P 12, Andreas Duerrmann**:** *Sterically Encumbered Coordination Sites. Iron(II) Complexes of Jäger-type ligands with a Terphenyl Backbone*

Tuesday, 31th of August:

9h-10h30, zoom session: to be defined

- Ming-Liang Tong : *Physical Stimuli and Chemical Modulations for Spin-Crossover Materials*
- Colette Bosckovic: *An Accurate and Convenient DFT-Based Strategy to Predict Transition Temperatures in Valence Tautomeric Molecular Switches*
- *Flash talks*
    - P 13, Jett Janetzki: *Dinuclear Fe(III) Complexes with Bridging Redox-Active Bis(dioxolene) Ligands for Multi-Step Spin Crossover*
    - P 14, Muhammad Nadeem*: Towards high-temperature light-induced spin-state trapping: insight from the crystal field theory and molecular dynamics*
    - P 15, Sriram Sundaresan: *Towards Predictable Tuning of Fe(II) Spin Crossover*
    - P16, Zahra Zahir: *A Simple DFT Approach for Predicting Transition Temperature in Valence Tautomeric Complexes*
    - P 17, Mamadou Ndiaye : *Competing Elastic Interactions and Generation of Self-organized spin states: Evidence of Symmetry Breaking*
    - P 18, Sakshi Mehta: : *Thermo and Photo-induced electron transfer in molecular model complexes of mixed-valence Fe^{III}/Fe^{II} Prussian Blue*

11h-12h30, zoom session: to be defined

- Xin Bao: *Thermo-, Acidity- and Photo-Driven Spin-State Switching in pyridylacylhydrazone Fe(II) Complexes*
- David Harding: *Turning on the Light in Iron(III) Spin Crossover Complexes*
- José Antonio Real: *Meltable Iron(II) Spin Crossover Complexes with Strong Cooperative Hysteretic Properties*

14h-16h, zoom session: to be defined

- *Introduction*
- Natia Frank: to be announced
- Yogendra Singh: *Spin Crossover Systems: Electro-elastic modelling and Multistep transition*
- Matvey Fedin: *Light-induced Spin State Switching in Copper-Nitroxide Magnets*
- Hans-Jörg Krüger*: to be announced*

Wednesday, 1st of September:

9h-10h30, zoom session: to be defined

- Masaaki Ohba : to be announced
- Jun Tao: *Switchable crystalline materials*
- Felix Tuczek: *Spin-state switching of iron complexes adsorbed on surfaces*

11h-12h30, zoom session: to be defined

- Vassilis Tangoulis: *Extreme Downsizing of Spin Crossover Nanoparticles Towards Stable Colloids in Water*
- Smail Triki: *Spin crossover in extended systems based on Fe(II) trinuclear units*
- Francisco Romero: *Interplay between spin crossover and hydrogen bonds in iron(II) compound*

Thursday, 2^{t} of September:

9h-10h30, zoom session: to be defined

- Sally Brooker : *Interesting correlations in spin crossover*
- Kazuyuki Takahashi: *Fundamentals and applications of molecular switches in metal coordination complexes from π-extended tridentate ligands*
- Hannah Kurz: *A Fluorescence-Detected Coordination-Induced Spin State Switch*

11h-12h30, zoom session: to be defined

- Mathieu Marchivie: *Contribution of X-ray Powder Diffraction to the Elaboration of full P/T Spin Crossover Materials Phase Diagrams : Re-investigation of the famous [Fe(PM-BiA)$_2$(NCS)$_2$] complex under pressure*
- Abhishake Mondal: *ON/OFF Photo(switching) and Crystal-to-Crystal Transformation in a 2D Hexagonal Network*
- Guillem Aromi: *Multifunctional Magnetic Devices through Designed Host-Guest Chemistry*

POSTERS

P 01 *Exploring the spin-crossover and conductive nature of heteroleptic Fe/Co complexes with redox-active phenalenol-substituted ligands*
Z. C. Watts, N. M. Bonanno, M. Pelaccia, A. Lough, B. Patrick, M. T. Lemaire.

P 02 *Influence of the magnetic field on the thermal activation barrier of spin-crossover materials*
T**. K. Ekanayaka,** G. Hao, A. T. N'Diaye, A. S. Dale, E. Mishra, X. Jiang, C. Mellinger, S. Yazdani, J. Freeland, J. Zhang, R. Cheng, X. Xu, P. A. Dowben

P 03 *Reversible Photo and Thermo-induced Spin-State Switching in a heterometallic {5d-3d} W_2Fe_2 Molecular Square Complex*
K. Kaushik, S. Ghosh, S. Kamilya, M. Rouzières, S. Mehta, A. Mondal

P 04 *Spin-crossover in iron (II) complexes with π-extended 2,2'-biimidazole ligands*
S. Yergeshbayeva, M. Shatruk

P 05 *Isotropic and anisotropic behavior in spin crossover molecular magnets through the mechanoelastic model.*
A.-I. Popa, L. Stoleriu, C. Enachescu

P 06 *A facile approach to prepare silica hybrid, spin crossover water-soluble nanoparticles as a potential platform for thermally responsive MRI agents*
P. Gkolfi

P 07 *3D spin crossover nanocrystals with operative bistable switching properties*
M. T. Delgado Perez

P 08 *Investigation of an Fe(II) SCO complex based on a heteroscorpionate ligand*
M. Pénicaud, M. Gonidec, P. Rosa

P 09 *Modulation of the fluorescence of polyfluorene with spin-crossover*
I. Sánchez-Molina, D. Nieto-Castro, A. Moneo-Corcuera, E. Martínez, J. R. Galán-Mascarós

P 10 *Smart molecular/MoS_2 heterostructures featuring light and thermally-induced strain driven by spin switching*
R. Torres-Cavanillas, M. Morant-Giner, G. Escorcia-Ariza, J. Dugay, J. Canet-Ferrer, S. Tatay, S. Cardona-Serra, M. Giménez Marqués, M. Galbiati, A. Forment-Aliaga, E. Coronado

P 11 *Investigation of the role of modulators in the synthesis of new Hofmann-type MOFs*
G. Truccolo, H. Shepherd

P 12 *Sterically Encumbered Coordination Sites. Iron(II) Complexes of Jäger-type ligands with a Terphenyl Backbone*
A. Duerrmann, B. Weber

P 13 *Dinuclear Fe(III) Complexes with Bridging Redox-Active Bis(dioxolene) Ligands for Multi-Step Spin Crossover*
J. T. Janetzki and Colette Boskovic

P 14 *Towards high-temperature light-induced spin-state trapping: insight from the crystal field theory and molecular dynamics*
M. Nadeem, J. Cruddas, G. Ruzzi, B.J. Powell

P 15 *Towards Predictable Tuning of Fe(II) Spin Crossover*
S. Sundaresan and S. Brooker

P 16 *A Simple DFT Approach for Predicting Transition Temperature in Valence Tautomeric Complexes*
F. Z. M. Zahir, J. T. Janetzki, R. W. Gable, L. Goerigk, C. Boskovic

P 17 *Competing Elastic Interactions and Generation of Self-organized spin states: Evidence of Symmetry Breaking*
M. Ndiaye, K. Boukheddaden

P18 *Thermo and Photo-induced electron transfer in molecular model complexes of mixed-valence Fe^{III}/Fe^{II} Prussian Blue*
S. Mehta, S. Kamilya, D. Li, D. Moon, R. Clérac, A. Mondal

P 19 *Fast, accurate enthalpy differences in spin crossover crystals from DFT+U*
M. Ohlrich, B. J. Powell

P 20 *Expanding Cobalt-based Valence Tautomerism to Alternative Redox-active Ligands*
M. A. Hay, J. T Janetzki, R. W. Gable, A. Starikova, C. Boskovic

P 21 *Synthesis and properties of pi-extended stable phenoxyl radical*
M. Wijesundara, N. Bonanno, A. Dmitrienko, M. Lemaire

P 22 *Wet-Chemistry Assembly of One-Dimensional Spin Crossover Nanowires/Nanorods and Study of Switching Characteristics through Raman Spectroscopy*
Z. G. Lada, A. Chrissanthopoulos, S. P. Perlepes, K. S. Andrikopoulos G. A. Voyiatzis

P 23 *Stepwise Spin-State Switching and Effect of Light Irradiation in Manganese(III) Complexes*
S. Ghosh, S. Bagchi, S. Kamilya, S. Mehta, A. Mondal

P 24 *Tuning of Spin Crossover Properties in a Series of Cobalt (II) Complexes based on Macrocyclic Tetradentate Ligand and Pseudohalide Co-ligands*
S. Kamilya, S. Ghosh, S. Selvamani, S. Mehta, A. Mondal

P 25 *Two-Step Thermo-Induced Metal-to-Metal Electron Transfer and ON/OFF Photo-Switching in a Molecular $[Fe_2Co_2]$ Square Complex*
M. Das, A. Mondal

P 26 *ON/OFF Photo-Switching and Thermo-Induced Spin Crossover with Cooperative Luminescence in 2D Iron(II) Coordination Polymer.*
S.M. Hossain, A. Mondal

P 27 *Synthesis of New Triazole-based Spin Crossover Materials and Implementation into Functional Devices*
D. Nieto-Castro, J. R. Galán-Mascarós

P 28 *Exploring the spin transition in gold@spin crossover heterostructures*
R. Sanchis, M. Gimenez

P 29 *Novel strategies in the design and synthesis of spin-crossover materials*
L. Birchall, H. Shepherd

P 30 *Asymmetric Ligand Design for Increased Volatility of Spin-Crossover Complexes*
M. Gakiya-Teruya, X. Jiang, A. Hebard, D. Le, T. Rahman, M. Shatruk

P 31 *Solvent-Dependent Spin Crossover Behavior of [Fe(Htrz)$_2$(trz)](BF$_4$)*
K. A. McElveen, R. Mahbub, T. K. Ekanayaka, E. Mishra, P. A. Dowben, R. Y. Lai

P 32 *Redox Amphoterism and Spin Crossover in TTF Based Iron (II) Complexes*
S. Schönfeld, B. Weber

P 33 *Thermal Switching and Related Macroscopic Deformations of Spin-Crossover Multi-layers*
N. Belmouri, K. Boukheddaden