Massine Kelai, 27 years old, Doctor in Physics

Education

September 2018 – March 2022 — **Doctoral degree, Quantum Materials and Phenomena Laboratory, University Paris Cité, Paris, France.**
Thesis title: *Switching and Magnetic Properties of Spin-Crossover Molecule/Metal Interfaces.*

September 2017 – July 2018 — **Master's degree** in Condensed Matter in the International Center for Fundamental Physics at **Ecole Normale Supérieur de Paris de Ulm, Paris, France.**

September 2016 – June 2017 — **Master's degree** in Fundamental Physics at **Sorbonne University, Paris, France.**

Teachings and Scientific Diffusion

2018 – 2021 — **Tutorials,** in Physics (Mechanics, electrostatic, ideal gases, hydrostatic in viscous media, waves, medical imaging) for the *first year common to health studies* (PACES), Medecine Department, University of Paris.

2019 – 2020 — **Tutorials,** in Second Year Bachelor in Electrostatics, Magnetostatics, Electrokinetics and Electromagnetism in Vacuum, Engineering Department, University of Paris.

2016 – 2019 — **Individual Tutoring,** in Mathematics and Physics for High School Students for a Private Company (*Complétude*: `https://www.completude.com/`), Paris, France.

2019 — **Public dissemination,** on Scanning Tunneling Microscopy in *Cité internationale universitaire de Paris* (`https://www.ciup.fr/`), International university residence, Paris, France.

Achievements: Research Publications

1. Tong, Y., Kelaï, M., Bairagi, K., Repain, V., Lagoute, J., Girard, Y., … Bellec, A. (2021). Voltage-Induced Bistability of Single Spin-Crossover Molecules in a Two-Dimensional Monolayer. *J. Phys. Chem. Lett.*, *12*(45), 11029–11034. doi:10.1021/acs.jpclett.1c03271
2. Kelai, M., Repain, V., Tauzin, A., Li, W., Girard, Y., Lagoute, J., … Bellec, A. (2021). Thermal Bistability of an Ultrathin Film of Iron(II) Spin-Crossover Molecules Directly Adsorbed on a Metal Surface. *J. Phys. Chem. Lett.*, *12*(26), 6152–6158. doi:10.1021/acs.jpclett.1c01366
3. Kelai, M., Cahier, B., Atanasov, M., Neese, F., Tong, Y., Zhang, L., … Mallah, T. (2021). Robust magnetic anisotropy of a monolayer of hexacoordinate Fe(II) complexes assembled on Cu(111). *Inorg. Chem. Front.*, *8*(9), 2395–2404. doi:10.1039/D1QI00085C

4 Zhang, L., Tong, Y., Kelai, M., Bellec, A., Lagoute, J., Chacon, C., … Repain, V. (2020). Anomalous Light-Induced Spin-State Switching for Iron(II) Spin-Crossover Molecules in Direct Contact with Metal Surfaces. *Angew. Chem. Int. Ed.*, *59*(32), 13341–13346. doi:10.1002/anie.202003896

Achievements: Communications

2021

Oral presentation to the french national meeting for condensed-matter physicist (*Journées de la Matière Condensée*, website: https://jmc17.sciencesconf.org/).
Presentation title: *Robust magnetic anisotropy of a monolayer of hexacoordinate Fe*(II) *complexes assembled on Cu(111).*
Oral presentation to the french national association of molecular magnetism (*Association Française de Magnétisme Moléculaire*, website: https://asso-am2.fr/conferences-am2/).
Presentation title: *Thermal Bistability of Iron(II) Spin-Crossover Molecules on a Metal.*

2020 and 2021

Invited speaker to the european research consortium project (*Concepts and tools in molecular spintronics (COSMICS)*, website: http://cosmics-h2020.eu/).
Presentation title in 2021: *Magnetic Coupling and Spin-State Blocking of Fe*(II) *Spin-Crossover with Ferromagnetic Surfaces.*
Presentation title in 2020: *Influence of the Molecular Thickness on the Thermal Transition of Fe*(II) *Spin-Crossover Complex Adsorbed on a Metal.*

2019

Oral presentation to the the french national research group of magnetism and molecular magnetism in (*GdR MCM-2 : Magnétisme et Commutation Moléculaires*, website: http://www.gdr-mcm2.cnrs.fr/).
Presentation title: *Anomalous Light-Induced Spin-State Switching for Fe*(II) *Spin-Crossover Molecules in Direct Contact with Metal Surfaces.*

Poster at Heidelberg (Germany) for the workshop on simulation of core-level spectroscopies, website: https://www.quanty.org/workshop/heidelberg.
Poster title: *Simulation of X-ray Absorption Spectra of* $Fe^{II}((3,5)\text{-}(CH_3)_2Pz)BH)_2$ *on different metals.*

Poster at Sologne (France) for the days of the quantum materials and phenomena laboratory.
Poster title: *Spin-Crossover Molecules on Metals.*

2018

Poster at Krakow (Poland) for the european school on magnetism, website: http://magnetism.eu/.
Poster title: *Structure and Magnetic Anisotropy of* $Fe^{II}((3,5)\text{-}(CH_3)_2Pz)BH)_2/Cu(111)$ *Interface.*

Summary of Ph.D. Work

- I am currently completing my final year of PhD thesis at the University of Paris in the *Laboratory of Quantum Materials and Phenomena* entitled ***Switching and Magnetic Properties of Spin-Crossover Molecule/Metal Interfaces.***
  During my thesis, I worked on thermal-, light-induced, electronic and magnetic properties of Iron(II) (Fe^{II}((3,5)-$(CH_3)_2$Pz)$BH)_2$) spin-crossover molecules deposited on metals, as well as on ferromagnetic surfaces. Among the contributions made during my PhD, I showed the modification of the optical absorption band and thermal-induced properties from assembled submonolayer to multilayers of spin-crossover molecules on metallic surfaces. In a few words, we demonstrated for the first time an anomalous switching behaviour under light for submonolayer coverages of molecules on nobel metals (Au(111), Cu(111) and Ag(111)), when the normal switching behavior is recovered above a certain thickness. An other achievement was to show, for the first time, the opening of a thermal hysteresis loop on a three-layered systems on Cu(111). On the latter substrate, I use the technique of scanning tunneling microscopy (STM) in which the switching of spin-transition molecules on Cu(111) and ferroelastic correlations between the molecules have been demonstrated under electric field. On magnetic substrates, namely Co/Cu(111) and Cu/Co/Cu(111), I also demonstrated the antiferromagnetic and ferromagnetic coupling between the later molecules and the substrates to achieve active spinterface. Therefore, this system is a suitable building block to design spintronic devices. Besides, I was involved in projects to highlight the change of the magnetic anisotropy of spin-crossover molecules and other single molecular magnets (based on Cobalt) on surfaces. To do so, I extensively worked in Synchrotron facilities (*SUN set – SOLEIL, DEIMOS beamline*, France) and my attention was particularly focused on X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD). To prepare my samples, I used standard ultrahigh vacuum techniques for substrate preparation (sputtering/annealing) and electron beam physical vapor deposition for the molecules. To check the high quality and cleanliness of the systems, I also used Auger spectroscopy and scanning tunneling microscopy. From a theoretical point of view, I also focused on the simulation of X-ray absorption spectra using *QUANTY* software (developed by HAVERKORT M., Heidelberg University) for Iron(II) complex in different crystal field symmetries. Furthermore, I master another software called PHI (developed by CHILTON N., Manchester University) to fit and calculate the magnetization curves obtained by XMCD for paramagnetic compound. Finally, I have also opened up to so-called *mechanoelastic* simulations using a Monte Carlo algorithm, in order to have a description of the ferroelastic interactions on surfaces and to have quantitative access to the dynamic properties under light and temperature of these systems and as a function of the system size.

Skills

Languages	Strong reading, writing and speaking competencies for English and Arabic. Mother tongues are French and Tamazight.
Coding	Python, C++ and LaTeX.
Other software	Origin Pro, Pack Office, Visual Studio, Audacity, Wordpress.

Hobbies

- Columnist and presenter of programs in an associative radio station (Radio Campus Paris).
  Writting french poetry.
  History and politics.