Personal Information

Name	KEPENEKIAN, Mikaël	**Email**	mikael.kepenekian@univ-rennes1.fr
Date of birth	25.04.1983	**Webpage**	https://perso.univ-rennes1.fr/mikael.kepenekian/

Current Situation

Since Oct. 2013 — **CNRS research fellow** (section 14)
Institut des Sciences Chimiques de Rennes UMR 6226 (Rennes, France)

Since July 2020 — **Associate vice-president of Université de Rennes for libraries and open science**

Education and Positions

Oct. 2019 — **Habilitation à Diriger des Recherches**
Université de Rennes 1, France

Oct. – Nov. 2016 — **Visiting scientist**
Centro de Física de Materiales (San Sebastian, Spain)

Jul. – Aug. 2014 — **Visiting scientist**
CINT, Los Alamos National Laboratory (Los Alamos, USA)

2010 – 2013 — **CSIC postdoctoral fellow**
Institut Catala de Nanociancia I Nanotecnologia (Bellaterra, Spain)
Host: Prof. N. Lorente

2007 – 2010 — **PhD in Theoretical Chemistry**
Commissariat à l'Energie Atomique (Grenoble, France)
École Normale Supérieure de Lyon (Lyon, France)
Advisors: Dr. P. Maldivi (CEA Grenoble) & Dr. V. Robert (ENS Lyon)
Title: "Ab initio inspection of magnetic and redox hysteresis"
Visiting student at Prof. K. Awaga's group (*Nagoya University*, Japan)
Gaston Berthier PhD award from the French Network for Theoretical Chemistry

2005 – 2007 — **Master degree in Material Sciences**
Ecole Normale Supérieure de Lyon (Lyon, France)

Scientific Production (from Web of Science™ on 15 December 2022)

Published publications	68	**Invited seminars**	9	***h*-index**	29
Book chapters	6	**Invited oral communications**	18	**Citations**	4018

The complete list of publications can be found at https://perso.univ-rennes1.fr/mikael.kepenekian/publications.html.

Skills and Interests – Molecules, Solids and Interfaces

Physical properties of materials for **optoelectronics** (*e.g.* halide perovskites)
Surface properties of **metals** and **semiconductors**
Transport properties of materials and molecules
Physico-chemistry of **magnetic and redox molecular systems**

Molecular and solid-state calculations based on density functional theory (**DFT**)
Description of excited states and out-of-equilibrium states through **Green's functions** formalism
Ab initio wavefunction-based **multireference** molecular calculations (CASSCF, CASPT2, DDCI)

Major National and International Collaborations

Prof. M. G. Kanatzidis	Department of Chemistry, Northwestern University, Northwestern (USA)
Prof. N. Mercier	*MOLTECH-Anjou*, Angers (France)
Prof. A. D. Mohite	Department of Materials Science and Nanoengineering, Rice University, Houston (USA)
Dr. C. Quarti	*Laboratoire de Chimie des Matériaux Nouveaux*, Mons (Belgium)

Granted Projects (Principal Investigator)

CNRS	**IEA**	**2022**	FRENCHFRIES (with Mons University)	20 k€ (CNRS: 10 k€, Mons: 10k€)
ANR	**PRC**	**2021**	MENIHR (Partner coordinator) MARCEL (Partner coordinator)	90 k€ 120 k€
CNRS	**Emergence@INC**	**2020**	ELDORaDOS	*ca.* 80 k€ (1-year postdoc & 15 k€)
GENCI	(HPC Grant)	**Since 2017**	Halides perovskites and cuprates	1 to 3 Mhours of cpu time per year
ANR	**JCJC**	**2015**	TRANSHYPERO	136 k€
CNRS	**PEPS**	**2014**	SOLHYBTRANS	15 k€
Rennes Métropole		**2014**	Simulation of molecular devices	40 k€

Granted Projects (Partner)

Horizon 2020 **FET Open 2020** PoLLoC, Coord: IBM Zurich (Switzerland) | **IA 2020** PeroCUBE, Coord.: CSEM, (Switzerland) | **FET Open 2019** DROP-IT, Coord.: University of Valencia (Spain) | **FET Open 2016** GOTSolar, Coord.: University of Porto (Portugal)

ANR **PRC 2019** HTHPCM, Coord.: Université de Rennes 1 (France) | **PRC 2018** MoreLess, Coord.: Université d'Angers (France) | **PRC 2015** SuperSansPlomb, Coord.: CEA Grenoble (France)

Institutional Responsibilities

Since 2020 **Associate vice-president for libraries and open science**, *Université de Rennes*
Leading a 72-people department managing a library network of 3 University Libraries (and annexes), ensuring the link with student education and research activities. Member of the office of the President. University representative to the 'Open science network' of *France Université*, the *Couperin consortium*, and the *Centre pour la Communication Scientifique Directe* of CNRS.

Since 2017 **Member of the scientific board** & **Webmaster**, *Groupement de Recherche CNRS HPero*
Contribution to the scientific life of the GDR including (i) budget distribution, (ii) attribution of mobility grants, (iii) organization of the annual conference of the GDR (*Journées des Pérovskites Halogénées*). Design and maintenance of the the GDR HPero website.

Since 2017 **Member of the scientific animation group**, *Institut des Sciences Chimiques de Rennes (ISCR)*
Organization of the annual ISCR seminar series. Organization of scientific events at the ISCR: Ethics and scientific integrity day (14 Nov. 2019), Open science day (26 Nov. 2021).

Since 2015 **Designer** and **webmaster** of the CTI group website, *ISCR*

2014 – 2021 **Elected member of the laboratory board** (Conseil d'Unité), *ISCR*

2018 – 2020 **Elected member of the board**, *Université de Rennes 1*

Advisor

Postdocs
N. Tymińska, Mar. 2020 – Mar. 2021
Metal and covalent organic frameworks based on organic radicals
B. Traore, Apr. 2017 – Oct. 2018
Bulks, surfaces and interfaces of halide perovskites

PhDs
B. Cucco (Director: 50%, Co-director: G. Volonakis: 50%), Started Nov. 2020
Computational design of novel 2D perovskite materials for energy applications
X. Che (Co-advisor: 50%, Director: J. Even: 50%), Oct. 2015 – Oct. 2018
Computational investigation of halide perovskites

M2 Students
A. Leduc (Co-supervisor with C. Quarti of Mons University), Mar. – Jul. 2021
Layered perovskites meet organic chromophores: electronic processes at the interface
T. Groizard (Co-supervisor with B. Le Guennic of ISCR), Feb. – Jul. 2015
Computational investigation of a gold-supported iron-based metal-organic framework

L3 Students (2-month internships)
G. Joalland (2022, *Layered halide perovskites*), N. Joubrel (2020, *Covalent organic frameworks*), P. Couacault (2019, *Metal-organic frameworks*), A. Bergonzoni (2018, *Halide perovskites*), X. Liu (2016, *Organic radicals*)

Teaching Activities

Since 2018	*École Nationale Supérieure de Chimie de Rennes*		
	Chemical bonding	L2	Lectures, tutorials & exam (54 h/year)
2014 – 2016	*Réseau Français de Chimie Théorique* (RFCT)		
	Introduction to electronic correlation	M2	Introductory lecture, 3 h/year
2007 – 2010	*Université Joseph Fourier* (now *Université Grenoble Alpes*), 64 h/year		
	Electronic structure background for chemistry	L3	practical sessions
	Physico-chemistry of colours	L1	lectures & practical sessions
	Physical chemistry	L1	lectures & practical sessions

Expertise activities

Juries	PhD Reviewer for F. Hleli (*Université d'Angers*), 14 Dec. 2022 PhD Reviewer for A. Mishra (*Université de Lorraine*), 28 Oct. 2021 PhD Examiner for J. Gosteau (*Université de Toulouse 3 Paul Sabatier*), 14 Oct. 2021 Examiner for an Associate Professor position at *École Normale Supérieure de Paris*, 2019
PhD monitoring	Member of 5 PhD monitoring committees (CSI) since 2019.
Reviewing	More than 210 articles (between 20 and 30 per year) mostly for Nature Publishing group (Nature, Nat. Commun., etc.), RSC (Energy Environ. Sci., Nanoscale, etc.), ACS (ACS Energy Lett., Chem. Mater., J. Phys. Chem. Lett., etc.), APS (Phys. Rev. Lett., Phys. Rev. Materials, etc.)
Project Expertise	ANR, Dutch Research Council (NWO), Department of Energy, Swiss National Science Foundation, Stanford Synchrotron Radiation Lightsource

Selected publications since 2013 (see details in the Report on research activities)

1. *Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites: from basics to devices*, M. Kepenekian, R. Robles, C. Katan, D. Sapori, L. Pedesseau, J. Even, *ACS Nano* **2015**, *12*, 11557 Open archive | CNRS commun.
2. *Enhanced Cooperativity in Supported Spin-Crossover Metal–Organic Frameworks*, T. Groizard, N. Papior, B. Le Guennic, V. Robert, M. Kepenekian, *J. Phys. Chem. Lett.* **2017**, *8*, 3415 Open archive
3. *Concept of lattice mismatch and emergence of surface states in 2D hybrid perovskite quantum wells*, M. Kepenekian, B. Traore, J.-C. Blancon, L. Pedesseau, H. Tsai, W. Nie, C. C. Stoumpos, M. G. Kanatzidis, J. Even, A. D. Mohite, S. Tretiak, C. Katan, *Nano Lett.* **2018**, *18*, 5603 Open archive
4. *Scaling law for excitons in 2D perovskite quantum wells*, J.-C. Blancon, A. V. Stier, H. Tsai, W. Nie, C. C. Stoumpos, B. Traore, L. Pedesseau, M. Kepenekian, F. Katsutani, G. T. Noe, J. Kono, S. Tretiak, S. A. Crooker, C. Katan, M. G. Kanatzidis, J. J. Crochet, J. Even, A. D. Mohite, *Nat. Commun.* **2018**, *9*, 2254 Open archive
5. *Charge trap formation and passivation in methylammonium lead tribromide*, X. Che, B. Traore, C. Katan, H.-H. Fang, M. A. Loi, J. Even, M. Kepenekian, *J. Phys. Chem. C* **2019**, *22*, 13812 Open archive
6. *Red-NIR luminescence of Mo_6 monolayered assembly directly anchored on Au(001)*, M. Kepenekian, Y. Molard, K. Costuas, P. Lemoine, R. Gautier, S. Ababou-Girard, B. Fabre, P. Turban, S. Cordier, *Mater. Horiz.* **2019**, *6*, 1828 Open archive
7. *Efficient and accurate calculation of band gaps of halide perovskites with the Tran-Blaha modified Becke-Johnson potential*, B. Traore, W. Lafargue-dit-Hauret, X. Rocquefelte, C. Katan, F. Tran, M. Kepenekian, *Phys. Rev. B* **2019**, *99*, 035139 Open archive
8. *Importance of vacancies and doping in hole transporting nickel oxide interface with halide perovskites*, B. Traore, L. Pedesseau, J.-C. Blancon, S. Tretiak, A. D. Mohite, J. Even, C. Katan, M. Kepenekian, *ACS Appl. Mater. Interfaces* **2020**, *12*, 6633 Open archive
9. *From 0D to 1D, opportunities and caveats of hybrid iodobismuthates for optoelectronic applications*, A. Skorokhod, N. Mercier, M. Allain, M. Manceau, C. Katan, M. Kepenekian, *Inorg. Chem.* **2021**, *60*, 17123 Open archive
10. *Tolerance Factor for Stabilizing 3D Hybrid Halide Perovskitoids Using Linear Diammonium Cations*, X. Li, M. Kepenekian, L. Li, H. Dong, C. C. Stoumpos, R. Seshradi, C. Katan, P. Guo, J. Even, M. G. Kanatzidis, *J. Am. Chem. Soc.* **2022**, *144*, 3902 Open archive