

PERSONAL INFORMATION

Name KEPENEKIAN, Mikael
Date of birth 25.04.1983
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CURRENT SITUATION

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

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 Nanociencia 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 SEPTEMBER 15, 2019)

Published publications	49	Invited seminars	8	h-index	21
Book chapters	6	Invited oral communications	14	Citations	1370

SKILLS AND INTERESTS – MOLECULES, SOLIDS AND INTERFACES

Physico-chemistry of **magnetic and redox molecular systems**

Surface properties of **metals** and **semiconductors**

Transport properties of materials and molecules

Physical properties of materials for **photovoltaics**

Ab initio wavefunction-based **multireference** molecular calculations (CASSCF, CASPT2, DDCI)

Molecular and periodic calculations based on density functional theory (**DFT**)

Description of excited states and out-of-equilibrium states through **Green's functions**

MAJOR INTERNATIONAL COLLABORATIONS

Combined theoretical and experimental approach to perovskite materials and devices

Los Alamos National Laboratory, Los Alamos (USA)

Dr. S. Tretiak

Rice University, Houston (USA)

Dr. A. D. Mohite

Northwestern University, Northwestern (USA)

Prof. M. G. Kanatzidis

Electronic transport in molecules and materials

Donostia International Physics Center, San Sebastian (Spain)

Prof. N. Lorente

Technical University of Denmark (DTU), Copenhagen (Denmark)

Dr. N. Papirer

SELECTED GRANTED PROJECTS

GENCI (HPC Grant)	Simulation of interfaces: hybrid perovskites/selective contact	Principal Investigator
	2018	1.3 Mhours of cpu time
	2017	1.1 Mhours of cpu time
	2016	330 khours of cpu time
H2020 – FET Open	GOTSolar	Partner
	2016 – 2019	85 k€ for ISCR
ANR – JCJC	TRANSHYPERO	Principal Investigator
	2015 – 2018	136 k€
CNRS – PEPS	SOLHYBTRANS	Principal Investigator
	2014	15 k€
Rennes Métropole	Simulation of molecular devices	Principal Investigator
	2014-2017	40 k€

INSTITUTIONAL RESPONSIBILITIES

Since 2018	<i>Université de Rennes 1</i> Elected member of the board
Since 2017	<i>Groupe de Recherche CNRS HPero</i> Member of the scientific board Webmaster of the GDR HPero website (http://gdr-hpero.cnrs.fr/)
Since 2017	<i>Institut des Sciences Chimiques de Rennes (ISCR)</i> Member of the scientific animation group
Since 2015	<i>Institut des Sciences Chimiques de Rennes (ISCR)</i> Designer and webmaster of the CTI group website (https://iscr.univ-rennes1.fr/cti/)
Since 2014	<i>Institut des Sciences Chimiques de Rennes (ISCR)</i> Elected member of the laboratory board (Conseil d'Unité)

ADVISOR

Apr. 2017 – Oct. 2018	B. Traore, Postdoc fellow Charge transport in perovskite-based devices through ab initio calculations
Oct. 2015 – Oct. 2018	X. Che, PhD student (co-advisor) DFT inspections of lead-free and colloidal halide hybrid perovskites
May – Jun. 2018	A. Bergonzoni, L3 student Initiation to computational studies of halide perovskite materials
May – Jun. 2016	X. Liu, L3 student Computational investigation of the bistability of grafted organic radicals
Feb. – Jul. 2015	T. Groizard, M2 student (co-advisor) DFT study of a self-organized metal-organic framework supported on Au(111)

TEACHING ACTIVITIES

Since 2018	<i>École Nationale Supérieure de Chimie de Rennes</i> Chemical bonding	L2	lectures & practical sessions
2014 – 2016	<i>Réseau Français de Chimie Théorique (RFCT)</i> Introduction to electronic correlation	M2	introductory lecture
2007 – 2010	<i>Université Joseph Fourier (Grenoble Alpes)</i> Electronic structure background for chemistry Physico-chemistry of colours Physical chemistry	L3 L1 L1	practical sessions lectures & practical sessions lectures & practical sessions

EVALUATION AND REVIEWING ACTIVITIES

Reviewing	More than 130 articles (26 in 2018) in Nature, J. Am. Chem. Soc., Nat. Commun., Nat. Nanotech., Energy Environ. Sci., ACS Energy Lett., Nanoscale, J. Phys. Chem. Lett., Nano Lett., Phys. Chem. Chem. Phys., Inorg. Chem., J. Phys. Chem. C, etc.
Project Expertise	ANR, Labex MiChem Sorbonne Universités, Labex NIE Strasbourg, Swiss National Science Foundation, Stanford Synchrotron Radiation Lightsource