#### **PERSONAL INFORMATION**

Name: Ian R. SIMS http://www.researcherid.com/rid/F-8989-2014 Born: 05/06/1963, Wimbledon, England. website: http://perso.univ-rennes1.fr/ian.sims/

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### **EDUCATION**

1985-1989 PhD in physical chemistry, University of Birmingham, UK (supervisor: Ian WM Smith: 'State selected kinetics of CN radical reactions')

1982-1985 BA/MA Natural Sciences (Chemistry), University of Cambridge, UK (St John's College)

## **CURRENT POSITION(S)**

2011-	Professeur des Universités Classe Exceptionnelle (Distinguished professor)	

- 2007-2011 Professeur des Universités Première Classe (Full professor)
- 2003-2007 Professeur des Universités 2ème Classe (Professor) at the Université de Rennes 1, Rennes, France (CNU section 30)

### PREVIOUS POSITIONS AND FELLOWSHIPS

- 1998-2003 Lecturer and Senior Lecturer (2001-) in Physical Chemistry at the School of Chemistry, University of Birmingham, UK
- 1993-1998 EPSRC Advanced Fellow at the School of Chemistry, University of Birmingham, UK
- 1991-1993 EU Postdoc / CNRS "Poste Rouge" at the Université de Rennes 1, France (Dr B.R. Rowe)
- 1989-1991 SERC-NATO Fellowship in the group of Professor Ahmed Zewail, Caltech, Pasadena, USA

#### **AWARDS**

- 2016-2021 Awarded ERC Advanced Grant (2.1 M €) for project CRESUCHIRP: Ultrasensitive Chirped-Pulse Fourier Transform mm-Wave Detection of Transient Species in Uniform Supersonic Flows for Reaction Kinetics Studies under Extreme Conditions
- 2012-2016 Award for Scientific Excellence (Prime d'Excellence Scientifique, P.E.S.)
- 2004-2008, Award for Research and Thesis Direction (Prime d'Encadrement Doctoral et de Recherche,
- 2008-2012 P.E.D.R.)
- 2013-14 6-month Research Sabbatical (CRCT) awarded by the University of Rennes 1
- 2012-13, Awarded three 6 month Research Sabbaticals (Délégations) by the CNRS
- 11-12, 8-9
- 2004-2007 EU Marie Curie Chair, held at the Université de Rennes 1 (awarded for project "Cool Chemistry Chemistry at Extremely Low Temperatures" € 416,000)
- 1993-1998 Awarded EPSRC Advanced Fellowship (held at the University of Birmingham, project "Ultra-Low Temperature Studies of Gas-Phase Reactions")
- 1989-1991 SERC-NATO fellowship to work with Prof. Ahmed Zewail (Nobel Prize, Chemistry, 1999)

### SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

- 2003-2018 Supervised 8 PhD students and 5 postdoctoral fellows Institut de Physique de Rennes, Université de Rennes 1, France. Currently supervising 3 postdocs and 3 PhD students.
- 1994-2003 Supervised 3 / co-supervised 3 PhD students; Directed 1 / co-directed 1 postdoctoral fellows School of Chemistry, University of Birmingham, UK.

## **TEACHING ACTIVITIES**

- Joint coordinator of new Master in Engineering Physics (Cursus Master en Ingénierie) awarded in national competition by the Figure Network (http://reseau-figure.fr)
- 2003- Lectures, tutorials and practical classes in physics (in French and English) at all levels from L1 to M2 and doctoral level.
- 1993-2003 Lectures, tutorials and practical classes in physical chemistry at all levels.

#### **INSTITUTIONAL RESPONSIBILITIES**

- 2016-2017 Director of Physical Sciences Doctoral School, Rennes (SDLM)
- 2010-2016 Assistant Director of Physical Sciences Doctoral School, Rennes (SDLM)
- 2008-2012 Assistant Director of the new Institut de Physique de Rennes (IPR)
- 2006-2008 Member of the Recruitment Committee (Commission de Spécialistes) for Physics at UR1

#### **COMMISSIONS OF TRUST**

- 2016- Member of Program Advisory Committee for Interdisciplinary Research (IPAC) beam time allocation panel for the GANIL accelerator
- 2014 Member of Evaluation Committee (HCERES: *Haut Conseil de l'Evaluation de la Recherche et de l'Enseignement Supérieur*) for LIPHY physics laboratory, Grenoble, France
- 2014 Member of Chemistry Evaluation Panel for COST (panel meeting in Brussels, Sep 2014)
- 2010-2018 Member of review panel for 'Chemical Dynamics / Gas Phase' program at the Berkeley Advanced Light Source Synchrotron
- 2009 Member of NASA grant panel for Laboratory Astrophysics (Washington DC, June 2009)
- 1997- External examiner (rapporteur) for 9 PhD theses and three HDR (Habilitation) theses
- 2003-2018 Reviewer for numerous grant proposals including ANR, NASA, NSF, ERC
- 1998-2003 Member of EPSRC Chemistry College, 1998-2001; Member EPSRC Structure, Bonding and Reaction Mechanisms Grant Awarding Panel, Jan/May 2000. Numerous referee reports.
- 1993-2018 Many reviews for journals inc Science, Nature Chem., JPC, JCP, PCCP, Angewandte, ApJ, etc

## **MEMBERSHIPS OF SCIENTIFIC SOCIETIES AND COMMITTEES**

RSC/RAS Astrophysical Chemistry Group, Secretary, 2002-2006, Chairman 2006-2010; RSC Gas Kinetics Discussion Group, Secretary 2004-2005, Chairman 2006-2007; Member of RSC Faraday Council, 2003-2006; Scientific Committee of the CNRS Interdisciplinary Programme 'Origin of Planets and of Life' 2007-2009.; Member of IAU Commission 34 / Division VI - Astrochemistry Working Group, 2009-2015.

#### MAJOR COLLABORATIONS AND NETWORKS

- 2017- International Research Network (GDRI) QUADMARTS on QUAntitative Detection of Molecular And Radical Trace Species produced by chemical reactions and photodissociation processes (with S.D. Le Picard and R. Georges).
- 2015- Mitchio Okumura (Caltech, Pasadena USA) 6 month research visit of Caltech PhD student Laura Mertens in 2015-16: 1 article published, 1 in preparation on energy transfer at low temperatures for astrophysics. 6 month research visit of Caltech PhD student Joey Messinger funded by NSF GROW project, March September 2019.
- 2015- Cecilia Ceccarelli, Paola Caselli and the SOLIS (Seeds of Life in Space) team: participation as expert on chemical reactivity in the gas phase. The SOLIS project aims to understand how, when and where interstellar complex organic molecules (iCOMs) form during the early stages of Solar-type star formation. SOLIS is a NOEMA Large Program.
- 2012- Arthur Suits (Wayne State, Detroit, USA, now U. Missouri) and Robert Field (MIT, Boston, USA) Development of Chirped-Pulse, FT mm-Wave Pulsed Uniform Supersonic Flow Spectrometer. Joint articles in JCP (two in 2014) and JPC Lett (2015)
- 2012- Millard Alexander (U. Maryland, USA) and François Lique (U. du Havre, France), leading theoreticians in the area of quantum scattering. Joint article in Nature Chemistry (2014)
- S.R. Leone, K.R. Wilson (UC Berkeley / Lawrence Berkeley Lab, USA) and D.L Osborn, C.A. Taatjes (Sandia National Lab, Livermore CA), award France Berkeley Fund grant of 10 000 \$
- 2010- Jean-Claude Guillemin, Ecole Nationale Supérieure de Chimie de Rennes, specialist in synthesis of unstable compounds of astrochemical interest. Joint EU FEDER grant.
- 2007-2011 R. Kaiser (U. Hawaii, USA), A. Mebel (Florida International U., Miami, USA), A. Suits (Wayne State, Detroit, USA). NSF Collaborative Research in Chemistry program *Titan: Observations, Experiments, Computations, and Modeling* (NSF 100 000 US \$ to Rennes)
- 2007- S.J. Klippenstein, Argonne National Laboratory, Chicago, IL, USA. SJK is world-leading theoretician in the area of chemical kinetics. Joint articles in Science (2007), J. Phys. Chem.

Lett. (2010), J. Phys. Chem. A. (2013)

2004-2008 Scientific Director for the Rennes team and President of the Board for the EC Marie Curie Research Training Network *The Molecular Universe* 

1997-2002 Network Co-ordinator for EC TMR Research Training Network Astrophysical Chemistry

# Section c: P.I.'s ten-year track record

## Ten representative publications since 2007

The P.I. is a corresponding author on all these.

- 1. H. Sabbah, L. Biennier, I. R. Sims, Y. Georgievskii, S. J. Klippenstein, and I. W. M. Smith, Understanding reactivity at very low temperatures: The reactions of oxygen atoms with alkenes, Science 317, 102 (2007).
- 2. F. Leonori, R. Petrucci, N. Balucani, P. Casavecchia, M. Rosi, D. Skouteris, C. Berteloite, S. D. Le Picard, A. Canosa, and I. R. Sims, Crossed-Beam Dynamics, Low-Temperature Kinetics, and Theoretical Studies of the Reaction S(¹D) + C<sub>2</sub>H<sub>4</sub> J. Phys. Chem. A 113, 15328 (2009).
- 3. C. Berteloite, M. Lara, A. Bergeat, S. D. Le Picard, F. Dayou, K. M. Hickson, A. Canosa, C. Naulin, J. M. Launay, I. R. Sims, and M. Costes, Kinetics and Dynamics of the S(¹D₂) + H₂ → SH + H Reaction at Very Low Temperatures and Collision Energies, Phys. Rev. Lett. 105, 203201 (2010).
- 4. C. Berteloite, S. D. Le Picard, N. Balucani, A. Canosa, and I. R. Sims, Low Temperature Rate Coefficients for Reactions of the Butadiynyl Radical, C<sub>4</sub>H, with Various Hydrocarbons. Part I: Reactions with Alkanes (CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>10</sub>), Phys. Chem. Chem. Phys. 12, 3666 (2010).
- 5. S. D. Le Picard, M. Tizniti, A. Canosa, I. R. Sims, and I. W. M. Smith, The Thermodynamics of the Elusive HO₃ Radical, Science 328, 1258 (2010).
- 6. H. Sabbah, L. Biennier, S. J. Klippenstein, I. R. Sims, and B. R. Rowe, Exploring the Role of PAHs in the Formation of Soot: Pyrene Dimerization, J. Phys. Chem. Lett. 1, 2962 (2010).
- S. B. Morales, C. J. Bennett, S. D. Le Picard, A. Canosa, I. R. Sims, B. J. Sun, P. H. Chen, A. H. H. Chang, V. V. Kislov, A. M. Mebel, X. Gu, F. Zhang, P. Maksyutenko, and R. I. Kaiser, A Crossed Molecular Beam, Low Temperature Kinetics, and Theoretical Investigation of the Reaction of the Cyano Radical (CN) with 1,3-Butadiene (C<sub>4</sub>H<sub>6</sub>) A Route to Complex Nitrogen-Bearing Molecules in Low Temperature Extraterrestrial Environments, Astrophys. J. 742, 26 (2011).
- 8. S. Cheikh Sid Ely, S. B. Morales, J. C. Guillemin, S. J. Klippenstein, and I. R. Sims, Low Temperature Rate Coefficients for the Reaction CN + HC₃N, J. Phys. Chem. A 117, 12155 (2013).
- 9. M. Tizniti, S. D. Le Picard, F. Lique, C. Berteloite, A. Canosa, M. H. Alexander, and I. R. Sims, Measurement of the rate of the F + H<sub>2</sub> reaction at very low temperatures Nature Chemistry 6, 141 (2014).
- 10. L. A. Mertens, H. Labiad, O. Denis-Alpizar, M. Fournier, D. Carty, S. D. Le Picard, T. Stoecklin, and I. R. Sims, Rotational energy transfer in collisions between CO and Ar at temperatures from 293 to 30 K, Chem. Phys. Lett. 683, 521 (2017).

# Invited presentations to peer-reviewed, internationally established conferences since 2006

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Date	Meeting
1. Jul 2018	Gordon RC on Molecular Interactions & Dynamics, Stonehill College, Easton MA USA
2. Apr 2018	Frontiers of Chemical Dynamics, Kavli Royal Society Centre, Chicheley Hall, UK
3. Mar 2018	Hydride chemistry: From earth to space, Telluride Science Research Center, CO, USA
4. Sept 2017	Astrochemical conference KIDA2017, Bordeaux, France
5. Sept 2017	David Williams 80th Birthday Conference, Royal Astronomical Society, London, UK
6. May 2017	10th International Conference on Chemical Kinetics, Chicago, Illinois, USA (Plenary)
7. Mar 2017	IAU Symposium 332: Astrochemistry VII – Through the Cosmos from Galaxies to Planets,
	Puerto Varas, Chile
8. Aug 2016	Physical Chemistry Meets AMO Symposium, 252nd National ACS Meeting, Philadelphia,
	Pennsylvania, USA
9. Mar 2016	Cold And Controlled Molecules and Ions, Weizmann Institute, Rehovot, Israel
10.Oct 2015	iCOMET 2015, Chengdu, China
11.Jul 2015	<b>Dynamics of Molecular Collisions XXV</b> , Celebrating 50 Years of Chemical Reaction Dynamics,
	Asilomar, California, USA
12.Apr 2015	Anharmonicity in medium-sized molecules and clusters, AMOC 2015, Madrid, Spain
13.Aug 2014	20th European Conference on Molecular Dynamics, MOLEC 2014, Gothenburg, Sweden

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14.Sep 2013	'Chemical Frontiers in Solar System Exploration' symposium at the 246th ACS National Meeting and Exposition, Indianapolis, Indiana, USA		
15.Jul 2013	32nd International Symposium on Free Radicals, Potsdam, Berlin, Germany		
16.Jul 2012	<b>Gordon</b> Research Conference on <b>Atomic and Molecular Interactions</b> , Stonehill College, Easton, MA, USA		
17.Sep 2011	First European Conference on Laboratory Astrophysics, Paris, France		
18.Sep 2011	<b>COMET 2011</b> International Conference on Molecular Energy Transfer, University of Oxford, UK		
19.Jul 2011	7th International Conference on Chemical Kinetics, MIT, Cambridge, MA, USA		
20.Feb 2011	Workshop on <b>Cold and Controlled Molecular Collisions</b> , Ringberg Castle near Lake Tegernsee, Germany		
21.Oct 2010	COST Action - <b>The Chemical Cosmos, First Annual Meeting</b> , Grenoble, France		
22.Mar 2010	'Recent Advances in Observational and Experimental Astrochemistry' symposium at 239 <sup>th</sup>		
22.10101 2010	ACS National Meeting, San Francisco, California, USA		
23.May 2007	International Astrophysics and Astrochemistry Conference 'Molecules in Space and		
-	Laboratory', Observatoire de Paris, France.		
24.Sep 2006	'Chemistry in Extreme Environments' symposium at the 232 <sup>nd</sup> ACS National Meeting, San		
	Francisco, CA, USA		
25.Jun 2006	Nobel Symposium on Cosmic Chemistry and Molecular Astrophysics, Stockholm, Sweden		
Organisation of international conferences in the field of the applicant (membership in the steering and/or			
organising committee (SOC / LOC)) since 2006			

organisation of international conferences in the field of the applicant (international the steering unit) or organising committee (SOC / LOC)) since 2006

Date Meeting Role

1	Date	Meeting	Role
1. 2	2017-	<i>Inaugural, First and Second Annual Network Meetings</i> of the QUADMARTS International Research Network	Co-organiser and member of SOC
2. J	Jun 2014	Mini-symposium on Spectroscopy in Kinetics and Dynamics, International Symposium on Molecular Spectroscopy, 69th Meeting, Champaign-Urbana, Illinois USA	Co-chair / convenor
_	2007- 2012	Six annual workshops on <i>Titan: Observations, Experiments, Computations, and Modeling</i> in Honolulu, HI, USA (2007); Miami, FL, USA (2008); San Juan, Puerto Rico (2009); St Jacut de la Mer France, (2010); Kauai, HI, USA (2011); Miami, FL, USA (2012)	Member of SOC
4.	Jun 2011	The Molecular Universe, IAU Symposium 280, Toledo, Spain	Member of SOC
5. J	Jun 2010	<i>Chemistry of the Planets,</i> Faraday Discussion 147, St Jacut-de-la-Mer, Bretagne, France	<b>Chair,</b> member of SOC and LOC
<b>6</b> . J	Jul 2008	20th International Symposium on Gas Kinetics, Manchester, UK	Member of SOC
	May 2007	International Astrophysics and Astrochemistry Conference 'Molecules in Space and Laboratory', Observatoire de Paris, France	Member of SOC (after being invited to speak!)
8. J	Jul 2006	19th International Symposium on Gas Kinetics, Orléans, France	Chair of SOC
9 /	Apr 2006	<i>Chemical Evolution in the Universe,</i> Faraday Discussion 133, St Jacut-de-la-Mer, Bretagne, France (also edited Discussion Volume published in November 2006)	

## Major contributions to the early careers of excellent researchers

September 2007: Dr David Carty, PhD directed by the PI 1999-2003, appointed to joint lectureship in the Departments of Physics and Chemistry of the University of Durham, UK, after postdoctoral fellowships in Berlin (Fritz Haber Institute, Prof. Gerard Meijer) and the University of Oxford (Prof T. Softley).

September 2011: Dr Hassan Sabbah, PhD directed by the PI 2005-8, is appointed to a lectureship in the Department of Physics at the Université Paul Sabatier, Toulouse, France after a postdoctoral fellowship with Prof R.N. Zare, Stanford University, USA