

CURRICULUM VITAE

RIADH SAHNOUN

Centre for Sustainable Nanomaterials
Ibnu Sina Institute for Scientific and Industrial Research
Universiti Teknologi Malaysia
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EDUCATION

- 09/1998 Ph.D. in Materials Science (option: Theoretical Chemistry).
National Polytechnic Institute, Graduate School of Chemical Engineering, Toulouse (France).
Supervisor: Prof. Claude Mijoule.
Topic: Dissociation process of organometallic compounds and simulation of the environment effects: a Density Functional Study – Application to $\text{Cr}(\text{C}_6\text{H}_6)_2$ and $\text{Ni}(\text{C}_5\text{H}_5)_2$.
- 09/1995 D.E.A. (Diploma of Advanced Studies, equivalent to Master's Degree) in Computational and Theoretical Chemistry.
Quantum Physics Laboratory at the Research Institute of Atomic and Molecular Complex Systems, (IRSAMC), Paul Sabatier University, Toulouse (France).
Supervisor: Prof. Colin J. Marsden.
Topic: Ab initio theoretical study of Lithium and Sulfur clusters: SLi_3 , SLi_3^+ and SLi_4^+ .
- 07/1994 A.E.A. (Diploma of Aptitude of Advanced Studies, equivalent to first year Master's Degree) in Solid State Chemistry.
University of Tunis, Tunis (Tunisia).
- 06/1993 Bachelor of Sciences in Physical Chemistry.
University of Tunis, Tunis (Tunisia).

EMPLOYMENT HISTORY

- 09/2010 – 12/2016 **Associate Professor**
Universiti Teknologi Malaysia, Johor Bahru (Malaysia).
- 06/2009 – 09/2010 **Assistant Professor**
Department of Chemistry, Science Faculty of Rabigh, King Abdul Aziz University, Rabigh (Saudi Arabia).
- 04/2007 – 03/2009 **Assistant Professor**
Department of Applied Chemistry, Graduate School of Engineering, Tohoku University, Sendai (Japan).
- 04/2006 – 03/2007 **Visiting Lecturer**
Department of Chemistry, School of Science and Engineering, Waseda University, Tokyo (Japan).
- 03/2005 – 04/2006 **Senior Research Engineer**
Institute of High Performance Computing, Singapore (Singapore).
- 11/2004 – 02/2005 **COE (Center of Excellence) Research Fellow**
Department of Chemistry, Graduate School of Science, Tohoku University, Sendai (Japan).
- 11/2002 – 10/2004 **JSPS Postdoctoral Research Fellow**
Department of Chemistry, Graduate School of Science, Tohoku University, Sendai (Japan).
- 01/2001 – 03/2002 **Postdoctoral Research Associate**
Institute for Physical and Theoretical Chemistry, Technical University of Munich, Munich (Germany).
- 04/2000 – 12/2000 **Postdoctoral Research Associate**
Laboratory of Organic Chemistry, Wageningen University, Wageningen (The Netherlands).

- 03/1999 – 03/2000 **Postdoctoral Research Associate**
Institute for Fundamental Chemistry [presently: Fukui Institute for Fundamental Chemistry, Kyoto University], Kyoto (Japan).
- 09/1995 – 07/1997 **Teaching Assistant “Atoms and Chemical Bonds”**
Tutorial for the third year undergraduate students in chemistry “Licence de Chimie”, Paul Sabatier University, Toulouse (France).

VISITING SCIENTIST

- 21/05/2012–25/05/2012 Visiting Professor, Dipartimento di Fisica, Sezione Struttura della Materia, Università degli Studi di Milano, Milan (Italy).
- 25/01/2010–29/01/2010 Visiting Professor, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru (Malaysia).

TEACHING EXPERIENCE

- A. Taught undergraduate courses at Universiti Teknologi Malaysia (UTM):
- Quantum Chemistry: SSCA 3463.
 - Quantum Chemistry and Spectroscopy: SSC 2463.
 - Symmetry and Molecular Spectroscopy: SSCC 2473.
 - Computer Literacy: SSH 1303.
 - Physical Chemistry Lab I: SSC 1841.
 - Physical Chemistry Lab II: SSC 2841.
- B. Taught undergraduate courses at King Abdul Aziz University:
- General Chemistry: CHEM 110.
 - General Chemistry Lab: CHEM 281.
- C. Taught undergraduate courses at Paul Sabatier University:
- Physical Chemistry Lab: Atoms and Chemical Bonds, including Point Groups Theory, Hückel Theory, Atomic and Molecular Spectroscopy (such as Infrared, Raman, Vibrational Spectroscopy, and Hydrogen Atom Spectrum), Magnetic Susceptibility Measurements, and Molecular Orbital Theory.

SUPERVISION

- 10/2015–Present Co-supervising Ms Siti Hajar Binti Alias, Doctor of Philosophy, Department of Chemistry, Universiti Teknologi Malaysia.
- 10/2015–Present Co-supervising Ms Nor Arbani Binti Sean, Master of Philosophy, Department of Chemistry, Universiti Teknologi Malaysia.
- 10/2015–Present Co-supervising Ms Nur Adilah Binti Hussien, Master of Philosophy, Department of Chemistry, Universiti Teknologi Malaysia.
- 03/2014–02/2017 Co-supervised Dr. Ai Ping Tan, Doctor of Philosophy, Department of Mathematics, Universiti Teknologi Malaysia.
- 01/2013–08/2016 Co-supervised Dr. Adam Mohammad Adam Bakheet, Doctor of Philosophy, Department of Physics, Universiti Teknologi Malaysia.
- 10/2015–05/2016 Supervised Ms Tharishinny Raja Mogan, Undergraduate Final Year Project, Department of Chemistry, Universiti Teknologi Malaysia.
- 01/2013–04/2016 Co-supervised Dr. Auwalu Musa, Doctor of Philosophy, Department of Physics, Universiti Teknologi Malaysia.
- 01/2011–11/2014 Supervised Dr. Alireza Zeinalinezhad, Doctor of Philosophy, Department of Chemistry, Universiti Teknologi Malaysia. *PhD awarded with A distinction.*
- 10/2012–06/2013 Supervised Mr Moh’d Kh. M. Abuelsheikh, Master of Philosophy, Department of Physics, Universiti Teknologi Malaysia.
- 04/2007–09/2008 Co-supervised a PhD student (Dr. A. Chutia), Graduate School of Engineering, Tohoku University.

- 04/2007–09/2008 Co-supervised a PhD student (Dr. Z. G. Zhu), Graduate School of Engineering, Tohoku University.
- 04/2007–09/2008 Co-supervised a PhD student (Dr. M. Ismael), Graduate School of Engineering, Tohoku University in Tohoku University.
- 04/2007–03/2009 Co-supervised a Research student (Ms. K. Ogiya), Graduate School of Engineering, Tohoku University in Tohoku University.
- 04/2007–03/2009 Co-supervised a Research student (Mrs. H. Malani), Graduate School of Engineering, Tohoku University in Tohoku University.
- 04/2007–03/2009 Co-supervised a PhD student (Dr. A. R. Shaikh), Graduate School of Engineering, Tohoku University in Tohoku University.
- 07/2005–04/2006 Supervised a Research Engineer (Dr. S. Abirami) in Institute of High Performance Computing, Singapore, for a project titled “Theoretical Investigation of Melanin”.
- 07/2005–02/2006 Supervised a trainee postgraduate student (Ms J. C. Kong from STMicronics Pte Ltd, Singapore) in IHPC, Singapore, for 8 months on subject related to the design of new quasicrystals.
- 11/2002–02/2005 Co-supervised a PhD student (Dr. K. Nakai), Graduate School of Science, Tohoku University.
- 11/2002–10/2003 Co-supervised an undergraduate student (Mr M. Sato), Graduate School of Science, Tohoku University.
- 04/2000–12/2000 Co-supervised an undergraduate student (Mr L. De Smet) during his probation, Wageningen University.

ACADEMIC AND PROFESSIONAL SERVICES

Service to University:

- 05/2011–04/2012 Principal Researcher in Ibnu Sina Institute for Fundamental Science Studies, UTM Johor.

Editorial boards:

- 03/2016–Present Editorial Board Member of “Malaysian Journal of Fundamental and Applied Sciences” Journal, Penerbit UTM Press, Universiti Teknologi Malaysia, Malaysia.
- 12/2012–01/2014 Lead Guest Editor of Special issue in “International Journal of Photoenergy”, Hindawi Publishing Corporation, New York, USA.
- 02/2012–Present Editorial Board Member of “Dataset Papers in Science” Journal, subject area: Physical Chemistry, Hindawi Publishing Corporation, New York, USA.

Reviewers:

- 2014–Present Journal of Physics and Chemistry of Solids
Journal of Organic Chemistry
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
Journal of Materials Science.
- 2011–Present Jurnal Teknologi.
- 2009–Present Journal of Physical Organic Chemistry.

Conference Committee Members:

- 01/2016–05/2016 Publication Committee Member for Indonesia-Malaysia Research Consortium Forum in conjunction with Regional Annual Fundamental Science Symposium 2016 (RAFSS 2016).
- 09/2015–05/2016 Technical Committee Member (International) for COMSOL MULTIPHYSIC Workshop held on 4–5 May 2016 at Ibnu Sina Institute, Universiti Teknologi Malaysia.

Professional Affiliations:

- 05/2013–05/2014 Membership of the American Association for the Advancement of Science, AAAS/Science (Member number 40900223).
- 09/2011–01/2014 Membership of the American Chemical Society (Member number: 30222230).
- 06/1999–06/2000 Membership of the Chemical Society of Japan.
- 1997–1998 Membership of the French Chemical Society.

UNIVERSITY COMMITTEES SERVICES

- 01/06/2011–31/05/2013 Committee Member of Research, Innovation & Consultation Undergraduate Research Program (UGRP) and Publication, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia.
- 01/06/2011–31/05/2013 Committee Member of Information Technology, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia.
- 01/06/2011–31/05/2013 Committee Member of Computational Unit, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia.
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RESEARCH GRANTS

Principal Investigator (Project Leader):

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|----|-----------------------|--|--------------|
| 3. | 01/06/2011–31/12/2012 | UTM Short Term Research Grant. | RM 30,000. |
| 2. | 01/04/2011–30/06/2013 | UTM-GUP Research University Grant Scheme. | RM 150,000. |
| 1. | 01/11/2002–31/10/2004 | JSPS Grant, served for purchasing local workstation and fees for participating in conference (inland and abroad) and for accessing the synergy supercomputer in Tohoku University. | ¥ 1,000,000. |

Co-Principal Investigator:

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|----|-----------------------|--|-------------|
| 5. | 01/03/2015–28/02/2016 | Flagship Research University Grant Scheme. | RM 50,000. |
| 4. | 01/12/2012–31/12/2014 | UTM-GUP Research University Grant Scheme. | RM 120,000. |
| 3. | 01/03/2012–31/03/2014 | MOHE-FRGS (Ministry of Higher Education, Malaysia) Research Grant. | RM 124,000. |
| 2. | 01/05/2012–30/04/2013 | UTM Research University Grant Scheme. | RM 30,000. |
| 1. | 01/04/2011–31/03/2013 | UTM-GUP Research University Grant Scheme. | RM 129,000. |
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COMPUTER SKILLS

- Operating System: Macintosh OS, UNIX, LINUX, MS-DOS and Windows environments.
 - Graphics (Sigma-Plot, Excel, PowerPoint...).
 - Chemical Editors (Molecule, Chemdraw, Chem3D, Molden, MolStudio...).
 - Scientific programs application
 - Gaussian G92, G94, G98, G03 and G09.
 - deMon.
 - HyperChem.
 - Gamess.
 - Cerius².
 - ParaGauss.
 - NWChem.
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RESEARCH INTERESTS

Scientific Theme: Quantum Chemistry

- 1) *Theoretical design of molecular catalysts with novel functions:*
 - Design of multi-metallic catalysts.
 - Reaction of small organic species at metal surfaces.
 - Catalytic cycle of organometallic catalysts and reaction dynamics.
 - Dissociation process of metallocene and arene compounds with and without external effects.
- 2) *Design and investigation of fundamental properties of materials exploited in solar cells:*
 - Excited state calculations of large molecular systems of technological interest (Dye Sensitized Solar Cells).
 - Theoretical investigation of fundamental properties of materials used in organic solar cells.

- 3) *Fullerenes:*
 - Stability of highly charged fullerenes and investigation of the effect of Laser field.
 - Encapsulation of H₂ inside fullerene cages.
 - Endohedral fullerenes: Encapsulation of transition metal inside fullerene cages.
- 4) *Quantum control of enantiomerization of chiral molecules.*
- 5) *Origin of conformational preference in several chiral derivatizing agents and molecules.*
- 6) *Electronic and optical properties of pure and doped β-tricalcium phosphate and Titanium dioxide Anatase.*

CITATION METRICS

	SCOPUS	WEB OF SCIENCE
Total	69	60
Overall Citation	783	739
Average Citation	11.35	12.32
H-index	16	15

For updates, see:

- <http://www.scopus.com/authid/detail.url?authorId=6603298645> for updates.
- http://apps.webofknowledge.com/summary.do?product=UA&parentProduct=UA&search_mode=CitationReport&parentQid=2&qid=3&SID=S1ZoB26OqsLAGs2ZIXn&&update_back2search_link_param=yes&page=1&action=sort&sortBy=TC.D;PY.D;AU.A.en;SO.A.en;VL.D;PG.A
- <http://orcid.org/0000-0003-1435-2579>
- <http://www.hindawi.com/51636747/>

REFEREED PUBLICATIONS

Scopus Author ID:6603298645, ISI Author ID: D-2266-2013, ORCID ID:0000-0003-1435-2579

International Journal Papers, Peer Reviewed Conference Papers and Book Chapters:

Title	IF(2015)	TC
81. A.-P. Tan, R. Sahnoun , S.-H. Yeak: "Improved Multi-scale Bond Stretching Model for the Diatomic Halogen Molecules", <i>Submitted</i> .	-	-
80. A.-P. Tan, R. Sahnoun , S.-H. Yeak: "Multi-scale Bond Stretching Model for the Diatomic Halogen Molecules", <i>Submitted</i> .	-	-
79. R. Sahnoun , N. Alias, M. Shamsuddin: "On the prediction of physical and chemical properties of benzene using MP4 method executed on high performance computing with homogenous platform", <i>Submitted</i> .	-	-
78. W. H. Danial, A. Chutia, Z. Abdul Majid, R. Sahnoun , M. Aziz: "Synthesis and Characterization of Stable Colloidal Solution of Graphene via Electrochemical Exfoliation", <i>Submitted</i> .	-	-
77. A. Zeinalinezhad, R. Sahnoun , V. P. Nambiar, M. Aziz: "Encapsulation of H ₂ and 2H ₂ Inside C ₅₀ Fullerene Cage: a HF, MP2 and DFT Comparative Study", <i>Submitted</i> .	-	-
76. M. M. Alsardia, M. A. Saeed, M. Yousaf, R. Sahnoun , A. Radzi Mat Isa: "Electronic structures and optical properties of XN (X=Al, Ga, B, In) compounds: A Density Functional Investigation", <i>Submitted</i>	-	-
75. N. Alias, R. Sahnoun , V. Malyskin: "High Performance Computing and Communication Models for Solving the Complex Interdisciplinary Problems on DPCS", <i>ARPN Journal of Engineering and Applied Sciences</i> , 12(2), 356–364 (2017). ISSN: 18196608	-	-
74. T. Ai-Ping, Y. Su-Hoe, R. Sahnoun : "Pristine Study of Axial Tension Strain Energy Curve for Single-Walled Carbon Nanotube using Molecular Dynamics Simulation", <i>Indian J. Sci. Technol.</i> , 3(28), 1–6 (2016). DOI: 10.17485/ijst/2016/v9i28/97775.	-	-
73. A. Musa, M. A. Saeed, A. Shaari, R. Sahnoun , M. Lawal, J. Munir: "Linear Acenes Linked Thiophene, Electronic and Chemical Properties: Prospects for Molecular Organic Electronic Material", <i>Jurnal Teknologi (Sciences & Engineering)</i> 78:6-11, 67–72 (2016). eISSN 2180–3722.	-	-
72. A. M. A. Bakheet, M. A. Saeed, A. R. M. Isa, R. Sahnoun : "Theoretical Investigations of β -Tricalcium Phosphate Biomaterials: DFT Insight", <i>Jurnal Teknologi (Sciences & Engineering)</i> 78:3-2, 159–164 (2016). eISSN 2180–3722.	-	-
71. A. M. A. Bakheet, M. A. Saeed, R. Sahnoun , A. R. M. Isa, L. Mohammed, T. Mahmood: "Density Functional Theory Study of the Electronic and Optical Properties of Pure and Magnesium Doped β -Tricalcium Phosphate Compound", <i>Jurnal Teknologi (Sciences & Engineering)</i> 78:3, 167–172 (2016). eISSN 2180–3722.	-	-
70. A. M. A. Bakheet, , M. A. Saeed, A. R. B. Mat Isa, R. Sahnoun : "First principles study of the physical properties of pure and doped calcium phosphate biomaterial for tissue engineering", in " <i>Nanobiomaterials in Hard Tissue Engineering, Applications of Nanobiomaterials</i> ", Ed. Alexandru Mihai Grumezescu, Vol. 4, pp. 215–240 (2016). Elsevier Inc., ISBN: 978-0-323-42862-0.	-	-
69. W. H. Danial, A. Chutia, Z. Abdul Majid, R. Sahnoun , M. Aziz: "Electrochemical Synthesis and Characterization of Stable Colloidal Suspension of Graphene Using Two-Electrode Cell System", Proceedings of The 23 rd Scientific Conference of Microscopy Society Malaysia (SCMSM 2014), Tronoh, Malaysia 10–12 December 2014, AIP Conference Proceeding 1669, 020020-1–7 (2015); http://dx.doi.org/10.1063/1.4919158 .	-	-
68. R. Sahnoun , A. Govindasamy, A. Miyamoto: "Efficiency enhancement of dye-sensitized TiO ₂ solar cell based on ruthenium(II) terpyridyl complex photosensitizer", <i>Int. J. Energy Res.</i> 39, 977–992 (2015). DOI: 10.1002/er.3308.	2.598	1
67. A. Musa, M. A. Saeed, A. Shaari, R. Sahnoun , M. Lawal: "Effects of delocalized π -electrons around the linear acenes ring (n= 1 to 7): an electronic properties through DFT and quantum chemical descriptors", <i>Mol. Phys.</i> , 113(11), 1347–1358 (2015). DOI: 10.1080/00268976.2014.993734.	1.870	0

66. W. H. Danial, A. Chutia, Z. Abdul Majid, **R. Sahnoun**, M. Aziz: “Electrochemical Synthesis and Characterization of Stable Colloidal Suspension of Graphene Using Two-Electrode Cell System”, *Malaysian Journal of Microscopy*, 10, 84–91 (2014). ISBN: 18237010.
65. V. P. Nambiar, M. Khalil-Hani, **R. Sahnoun**, M. N. Marsono: “Hardware Implementation of Evolvable Block-Based Neural Networks Utilizing a Cost Efficient Sigmoid-Like Activation Function”. *Neurocomputing*, 140, 228–241 (2014). DOI: 10.1016/j.neucom.2014.03.018.
64. A. Zeinalinezhad, **R. Sahnoun**, V. P. Nambiar, M. Aziz: “An MP2 Investigation on the Encapsulation of H₂ and 2H₂ Inside C₅₀ Fullerene”, *Chem. Phys. Lett.*, 594(58), 58–63 (2014). DOI: 10.1016/j.cplett.2014.01.024.
63. A. Zeinalinezhad, **R. Sahnoun**, M. Aziz: “Ab Initio Molecular Orbitals Studies and NBO Analysis of Conformational Preference in 2-Hydroxypiperidine”, *Comput. Theor. Chem.*, 1024, 52–60 (2013). DOI: 10.1016/j.comptc.2013.09.012.
62. A. Chutia, **R. Sahnoun**, R. C. Deka, Z. Zhu, H. Tsuboi, H. Takaba, A. Miyamoto: “Local electronic and electrical properties of functionalized graphene nano flakes”, *Physica B: Condensed Matter*, 406(9), 1665–1672 (2011). DOI: 10.1016/j.physb.2010.01.012.
61. T. Onodera, Y. Morita, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, R. Deka, M. Kubo, A. Miyamoto: “Tribochemical reaction dynamics of molybdenum dithiocarbamate on nascent Iron surface: A hybrid quantum chemical/classical molecular dynamics study”, *J. Nanosci. Nanotechnol.*, 10(4), 2495–2502 (2010). DOI: 10.1166/jnn.2010.1399.
60. C. Lv, K. Ogiya, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, R. Deka, M. Kubo, A. Miyamoto: “Quantum chemistry study on absorption spectra, electronic and electrical properties of organic dye on anatase (001)”, *J. Nanosci. Nanotechnol.*, 10(4), 2434–2443 (2010). DOI: 10.1166/jnn.2010.1398.
59. H. Onuma, H. Tanno, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, M. Kubo, R. C. Deka, H. Kajiyama, T. Shinoda, A. Miyamoto: “Host Emission from BaMgAl₁₀O₁₇ and SrMgAl₁₀O₁₇ Phosphor: Effects of temperature and defect level”, *J. Soc. Inf. Display*, 18(3), 211–222 (2010). DOI: 10.1889/JSID18.3.211.
58. K. K. Sahu, M. Ismael, S. M. A. Rauf, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, R. C. Deka, C. A. Del Carpio, M. Kubo, A. Miyamoto: “Applying ultra accelerated quantum chemical molecular dynamics technique for the evaluation of ligand protein interactions”, *Med. Chem. Res.*, 19(1), 1–10 (2010). DOI: 10.1007/s00044-009-9167-y.
57. Y. Morita, T. Onodera, T. Kuriaki, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, M. Kubo, A. Miyamoto: “Effect of misfit angle on superlubricity of molybdenum disulfide: A computational chemistry study”, *World Tribology Congress 2009–Proceedings*, Kyoto; Japan; 6-11 September 2009, pp. 258 (2009).
56. **R. Sahnoun**, Y. Fujimura, K. Kabuto, Y. Takeuchi, R. Noyori: “Substituent effects on conformational preference in α -substituted α -fluorophenylacetic acid methyl ester model systems for chiral derivatizing agents”, *J. Phys. Org. Chem.*, 22(10), 903–912 (2009). DOI: 10.1002/poc.1537.
55. S. M. AbdurRauf, M. Ismael, K. K. Sahu, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, M. Kubo, A. Miyamoto: “A graph theoretical approach to the effect of mutation on the flexibility of the DNA binding domain of p53 protein”, *Chem. Pap.*, 63(6), 654–661 (2009). DOI: 10.2478/s11696-009-0068-9.
54. M. Ismael, **R. Sahnoun**, A. Suzuki, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, M. Kubo, S. Shimizu, C. A. Del Carpio, A. Miyamoto: “A DFT study on the carbamates formation through the absorption of CO₂ by AMP”, *Int. J. Greenh. Gas Control*, 3(5), 612–616 (2009). DOI: 10.1016/j.ijggc.2009.04.002.

53. Z. Zhu, R. C. Deka, A. Chutia, **R. Sahnoun**, H. Tsuboi, M. Koyama, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, M. Kubo, A. Miyamoto: “Enhanced gas-sensing Behavior of Ru doped SnO₂ surface: A periodic density functional approach”, *J. Phys. Chem. Solids*, 70(9), 1248–1255 (2009). DOI: 10.1016/j.jpcs.2009.07.012. 2.059 26
52. H. Tsuboi, A. Chutia, C. Lv, Z. Zhu, H. Onuma, R. Miura, A. Suzuki, **R. Sahnoun**, M. Koyama, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, R. C. Deka, M. Kubo, A. Miyamoto: “An electrical conductivity prediction simulator based on TB-QCMD and KMC. System development and applications”, *J. Mol. Struct.–Theochem*, 903(1-3), 11–22 (2009). DOI: 10.1016/j.theochem.2008.11.040. 1.371 4
51. H. Malani, S. Hayashi, A. Suzuki, **R. Sahnoun**, H. Tsuboi, M. Koyama, N. Hatakeyama, A. Endou, H. Takaba, M. Kubo, C. A. Del Carpio, A. Miyamoto: “Ultra accelerated quantum chemical molecular dynamics study on ethylene polymerization reaction using CpSiH₂NHTiCl₂-Constrained geometry catalyst”, *Top. Catal.*, 52(6-7), 724–730 (2009). DOI: 10.1007/s11244-009-9210-8. 2.486 2
50. M. K. Alam, F. Ahmed, K. Nakamura, A. Suzuki, **R. Sahnoun**, H. Tsuboi, M. Koyama, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, M. Kubo, A. Miyamoto: “Study of carbon monoxide oxidation on CeO₂(111) using ultra accelerated quantum chemical molecular dynamics”, *J. Phys. Chem. C*, 113(18), 7723–7727 (2009). DOI: 10.1021/jp8088963. 4.536 32
49. H. Tsuboi, M. Kabasawa, S. Ouchi, M. Sato, **R. Sahnoun**, M. Koyama, N. Hatakeyama, A. Endou, H. Takaba, M. Kubo, C. A. Del Carpio, Y. Kitou, E. Makino, N. Hosokawa, J. Hasegawa, S. Onda, A. Miyamoto: “Computational evaluation of electrical conductivity on SiC and the influence of crystal defects”, *Silicon carbide and related materials 2007*, pts 1 and 2. Eds. A. Suzuki, H. Okumura, T. Kimoto, T. Fuyuki, K. Fukuda, S. Nishizawa. Book series: *Materials Science Forum*, 600-603, 497–500 (2009). ISSN: 0255-5476, DOI: 10.4028/3-908453-11-9. 0.399 3
48. H. Takaba, A. Sagawa, M. Sato, S. Ouchi, Y. Yoshida, Y. Hayashi, E. Sato, K. Inaba, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, M. Kubo, C. A. Del Carpio, Y. Kitou, E. Makino, N. Hosokawa, J. Hasegawa, S. Onda, A. Miyamoto: “Multi-level simulation study of crystal growth and defect formation processes in SiC”, *Silicon carbide and related materials 2007*, pts 1 and 2. Eds. A. Suzuki, H. Okumura, T. Kimoto, T. Fuyuki, K. Fukuda, S. Nishizawa. Book series title: *Materials Science Forum*, 600-603, pp. 131–134(2009). ISSN: 0255-5476, DOI: 10.4028/3-908453-11-9.131. 0.399 0
47. K. Ogiya, C. Lv, A. Suzuki, **R. Sahnoun**, M. Koyama, H. Tsuboi, N. Hatakeyama, A. Endou, H. Takaba, C. A. Del Carpio, R. C. Deka, M. Kubo, A. Miyamoto: “Simulation of electron diffusion in TiO₂ porous structures in dye-sensitized solar cells”, *Jpn. J. Appl. Phys.*, 48(4), 04C166-1–5 (2009). DOI: 10.1143/JJAP.48.04C166. 1.384 3
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Papers Ready for Submission:

- R. Sahnoun**, V. P. Nambiar, P. Wu:
Theoretical Design of Binary Decagonal Raney-type Quasicrystal.
- R. Sahnoun**, H. Zuilhof:
Density Functional and *ab initio* Molecular Orbitals Studies of Diacetylene Oligomers.

Papers in Preparation:

- A. Zeinalinezhad, **R. Sahnoun**, M. Aziz:
Ab initio molecular orbital and DFT investigation on the encapsulation of H₂ molecules inside C₇₈.
- R. Sahnoun**, A. Zeinalinezhad, M. Aziz:
Why only one H₂ molecule can be encapsulated inside C₆₀ Fullerene? A theoretical evidence.
- R. Sahnoun**, A. Zeinalinezhad:
Ab initio molecular orbitals study of the conformational preference in 2-aminoacetaldehyde and methyl 2-aminoacetate.
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 ORAL COMMUNICATIONS-CONFERENCES-WORKSHOPS

Plenary Lecture

1. **R. Sahnoun**: “Endohedral hydrogen fullerenes: where theoretical calculations are in line with experimental results” Second Polish-Taiwanese Conference “From Molecular Modeling to Nano- and Biotechnology”, August 26–28, 2015, Opole-Groszowice, Poland.

Invited Speaker

2. **R. Sahnoun**: “Quantum Chemistry Methods: Basics and Performance” and “Examples Illustrating Some of Physical and Chemical Properties Obtained From Computational Chemistry” Computational Science Workshop, Ibnu Sina Institute for Fundamental Science Studies (IIS), December 6–10, 2010, Universiti Teknologi Malaysia, Johor Bahru, Malaysia.
1. **R. Sahnoun**, K. Kabuto, Y. Takeuchi, Y. Fujimura, R. Noyori: “Toward Understanding the Conformational Preference in α -Cyano- α -fluoro-*p*-tolyl-acetic Acid Derivatives: An ab initio Molecular Orbital Study”, International Fluorine Conference in Toyama, Toyama International Conference Center, **I05**, pp 13–15, November 1–2, 2005, Toyama, Japan.

International Conferences, Symposiums and Workshops

16. T. Ai-Ping, Y. Su-Hoe, **R. Sahnoun**: “Pristine Study of Axial Tension Strain Energy Curve for Single-Walled Carbon Nanotube using Molecular Dynamics Simulation”, ICCSCM-2016, Universiti Teknologi Malaysia. May 5–6, 2016, Langkawi, Malaysia.
15. T. Ai-Ping, Y. Su-Hoe, **R. Sahnoun**: “Bond Stretching Model for the Diatomic Molecules”, AIP Proceeding series, SKSM23, pp73, November 24–26, 2015, Universiti Teknologi Malaysia, Malaysia
14. N. Alias, **R. Sahnoun**, V. Malyskin: “High Performance Computing and Communication Models for Solving the Complex Interdisciplinary Problems on DPCS”, Proceeding of The 1st International Conference on Science, Technology and Interdisciplinary Research 2015, IC-STAR 2015, pp.72, Bandar Lampung, September 23–25, 2015, Eds. D. Kurniawan, T. Adiono, Warsito, D. Suhandy, D. Noviana, Publisher: UPT. Perpustakaan Universitas Lampung, ISBN: 978-602-73260-0-2.
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12. **R. Sahnoun**, H. Nakai: “Quantitative Evaluation of the Hyperconjugation for Polyacetylene Methyl Rotation”, The 4th 21COE International Symposium on “Practical Nano-Chemistry”, Waseda University International Conference Center, P47, pp75, December 11–12, 2006, Tokyo, Japan.
11. **R. Sahnoun**, J. C. Kong, Y. Zeng, P. Wu: “On the Design of Raney-Type Catalysts: A Density Functional Study”, 6th Canadian Computational Chemistry Conference, University of British Columbia, July 26–30, 2006, Vancouver, British Columbia, Canada.
10. **R. Sahnoun**: “Stability of Highly Charged Fullerene: A DFT Study”, International Workshop on First-Principle Quantum Methods and Applications to Dynamical Processes, Department of Chemistry, Graduate School of Science, Tohoku University, October 12, 2004, Sendai, Japan.
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4. I. V. Yudanov, **R. Sahnoun**, **K. M. Neyman**, N. Rösch: “CO adsorption on Pd nanoclusters: Density functional PARAGAUSS studies”, Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Deutsche Forschungsgemeinschaft, May 21–22, 2001, Berlin, Germany.
3. I. V. Yudanov, S. Hengrasme, **R. Sahnoun**, **K. M. Neyman**, N. Rösch: “Electronic Structure of Mixed Pd/Zn Systems”, Priority Program 1091 “From Ideal to Real Systems: Bridging the Pressure and Material Gap in Heterogeneous Catalysis”, Deutsche Forschungsgemeinschaft, May 21–22, 2001, Berlin, Germany.
2. **R. Sahnoun**, T. Matsubara, N. Koga, T. Yamabe: “Density Functional Study of the Mechanism of the Stannole Formation Catalyzed by Transition Metal Complexes”, 8th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics, DFT 99, September 6–10, 1999, Rome, Italy.
1. **R. Sahnoun**, C. Mijoule: “Density Functional Study of Transition Metal Benzene and Cyclopentadienyl Complexes: Dissociation Energies of Cr(C₆H₆)₂, Cr(C₆H₆), Ni(C₅H₅) and Ni(C₅H₅)₂”, 7th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics, DFT 97, pp 62, September 2–6, 1997, Vienna, Austria.

Domestic Symposiums and Workshops

13. **R. Sahnoun**, A. Govindasamy, M. Koyama, H. Tsuboi, N. Hatakeyama, H. Takaba, M. Kubo, C. A. Del Carpio, A. Miyamoto: “Ligand Effects on the Enhancement of the Photophysical Properties of Black Dye Sensitizer for TiO₂ Based Solar Cells: A Theoretical Investigation”, 100th Catalysis Society Meeting of Japan, CATSJ100, 4I03, pp 375, Hokkaido University, September 19–20, 2007, Sapporo, Japan.
12. **R. Sahnoun**, H. Nakai: “Theoretical Evidence of Hyperconjugation for Polyacetylene Methyl Rotation”, SCCJ2006, Society of Computer Chemistry of Japan, Hokkaido University of Education, O2002, October 14–15, 2006, Hakodate, Japan.
11. **R. Sahnoun**, H. Kono, Y. Fujimura: “Highly Charged States of C₆₀ Molecule: a DFT Study”, Proceedings of Molecular Structure Conference 2004, 3P128, September 27–30, 2004, Hiroshima, Japan.
10. **K. Nakai**, T. Kato, **R. Sahnoun**, H. Kono, Y. Fujimura: “TDDFT Investigation of the Charge Transfer State of meso,meso-Linked Porphyrin Dimer”, Proceedings of Molecular Structure Conference 2004, 3P120, September 27–30, 2004, Hiroshima, Japan.
9. **R. Sahnoun**, K. Kabuto, Y. Takeuchi, Y. Fujimura, R. Noyori: “A Theoretical Investigation of the Conformational Preference in α -Cyano- α -Fluorophenylacetic Acid Model Systems: the Important Role of Hyperconjugation”, 17th Symposium on Fundamental Organic Chemistry, September 23–25, 2004, Sendai, Japan.
8. **R. Sahnoun**, S. Koseki, Y. Fujimura: “Theoretical Investigation of the Dynamics of the Binaphthol Isomerization”, Proceedings of Molecular Structure Conference 2003, 4Pa005, September 24–27, 2003, Kyoto, Japan.
7. **K. Nakai**, T. Kato, **R. Sahnoun**, H. Kono, Y. Fujimura: “Electric Field Induced Charge Transfer of Porphyrin Array”, Proceedings of Molecular Structure Conference 2003, 4Pa070, September 24–27, 2003, Kyoto, Japan.
6. **M. Sato**, M. Yamaki, K. Hoki, **R. Sahnoun**, L. González, Y. Otsuki, S. Koseki, Y. Fujimura: “Theoretical Design Using the Electronic Excitation State of a Molecule Motor”, 83rd annual meeting, 1PB-167, March 18–23, 2003, Waseda University, Tokyo, Japan.
5. **R. Sahnoun**, T. Matsubara, N. Koga, T. Yamabe: “Density Functional Study of Stannole Synthesis Catalyzed by Transition Metal Complexes”, Symposium on Molecular Structure, 3pB17, September 27–30, 1999, Osaka University, Osaka, Japan.

4. **R. Sahnoun**, T. Matsubara, N. Koga, T. Yamabe: “Mechanistic Aspects of the Stannole Formation Catalyzed by Transition Metal Complexes: A Density Functional Study”, 46th Symposium on Organometallic Chemistry, Kinki Chemical Society, PA220, pp 166–167, September 16–17, 1999, Osaka, Japan.
3. **R. Sahnoun**, C. Mijoule: “A Density Functional Study of the Dissociation Process of Nickelocene”, 8th Chemical Workshop of the Southwest Part of France, French Chemical Society, pp C702, November 27, 1998, University of Pau, Pau, France.
2. **R. Sahnoun**, C. Mijoule: “Effects of the Temperature on the Bond Dissociation Energy of Bis(Benzene)Chromium Cation”, Workshop of Young Scientists, French Chemical Society, April 29, 1998, INP-ENSCT, Toulouse, France.
1. **R. Sahnoun**, C. Mijoule: “Electric Field Effects on the Bond Dissociation Energies of Several Organometallic Compounds: a Density Functional Study”, Workshop of Young Scientists, French Chemical Society, May 29, 1997, INP-ENSCT, Toulouse, France.

INVITED SEMINARS

9. “Theoretical Evidence that Hyperconjugation is Responsible for the Conformational Preference in α -Cyano- α -Fluoro- p -Tolylacetic Acid Analogues”, May 24, **2012**, Dipartimento di Fisica, Sezione Struttura della Materia, Università degli Studi di Milano, Milan, Italy.
8. “Quantum Chemistry: Challenges and Opportunities”, January 27, **2010**, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru, Malaysia.
7. “An Overview on the Application of Theoretical Methods to Problem Related to Chemistry, Physics and Materials Science”, February 21, **2009**, Department of Applied Physics, Center for Research and Development of Higher Education, The University of Tokyo, Tokyo, Japan.
6. “Introduction to Computational Chemistry”, Ritsumeikan Asia Pacific University, March 21, **2008**, Beppu, Oita, Japan.
5. Part A: “Theoretical Investigation of the Dynamics of the Binaphthol Isomerization”,
and
Part B: “A Theoretical Investigation of the Conformational Preference in α -Cyano- α -Fluorophenylacetic acid Model Systems: the Important Role of Hyperconjugation”, August 27, **2004**, Institute for Molecular Science (IMS), Okazaki, Japan.
4. Part A: “Dissociation Process of Bis(Benzene)Chromium and its Cation: a Density Functional Study”,
and
Part B: “Density Functional and ab initio Molecular Orbital Studies of Diacetylene Oligomers”, Laboratoire de Chimie Théorique Appliquée, Facultés Universitaires Notre-Dame de la Paix (FUNDP), December 3, **2001**, Namur, Belgium.
3. “Density Functional and ab initio Molecular Orbital Studies of Diacetylene Oligomers”, Institut für Physikalische und Theoretische Chemie, Technische Universität München, November 3, **2000**, Munich, Germany.
2. “Quantum Chemistry from Theory to Application: the Density Functional Method”, Chemistry and Physics Departments, March 3, **1999**, University of Sfax, Sfax, Tunisia.
1. “Dissociation Process of $\text{Cr}(\text{C}_6\text{H}_6)_2$ and Simulation of the Effects of Metallic Surface: A Density Functional Study”, Laboratoire de Chimie de Coordination, November 24, **1998**, Toulouse, France.

AWARDS AND RECOGNITIONS

- Received numerous invitations as *Plenary Lecturer*, *Invited Speaker*, *Invited Editor*, *Lead Guest Editor* for special issues, *Reviewer*, and *Conference Organizer* but have been declined.
- **Visiting Professor**, May 21–24, 2012, Dipartimento di Fisica, Sezione Struttura della Materia, Università degli Studi di Milano, Milan, Italy.
- **Invited Speaker** in “Computational Science Workshop”, Ibnu Sina Institute for Fundamental Science Studies (IIS), December 6–10, 2010, Universiti Teknologi Malaysia, Johor Bahru, Malaysia.
- **Visiting Professor**, January 27, 2010, Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru, Malaysia.

- **Invited seminar**, February 21, 2009, Department of Applied Physics, Center for Research and Development of Higher Education, The University of Tokyo, Tokyo, Japan.
- **Paper Award**, Society of Computer Chemistry, Japan, May 22, 2008: “Development of Three-Dimensional Porous Structure Simulator POCO² for Simulations of Irregular Porous Materials”, Michihisa Koyama, Kei Ogiya, Tatsuya Hattori, Hiroshi Fukunaga, Ai Suzuki, **Riadh Sahnoun**, Hideyuki Tsuboi, Nozomu Hatakeyama, Akira Endou, Hiromitsu Takaba, Momoji Kubo, Carlos A. Del Carpio, and Akira Miyamoto.
- **Invited seminar**, March 21, 2008, Ritsumeikan Asia Pacific University, Beppu, Oita, Japan.
- **Visiting Lecturer**, April 2006, Department of Chemistry, School of Science and Engineering, Waseda University, Tokyo, Japan.
- *Paper selected by editors: J. Chem. Phys.*, 125, 184306-1–10 (2006).
- *Paper selected by editors: B. Chem. Soc. Jpn.*, 79, 555–560 (2006).
- **Invited speaker** in “International Fluorine Conference in Toyama”, Toyama International Conference Center, November 1–2, 2005, Toyama, Japan.
- **COE (Center of Excellence) Research Fellow**, November 2004, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, Japan.
- **Invited seminar**, August 27, 2004, Institute for Molecular Science (IMS), Okazaki, Japan.
- **JSPS Postdoctoral Research Fellow Award**, November 2002, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, Japan.
- **Invited seminar**, December 3, 2001, Laboratoire de Chimie Théorique Appliquée, Facultés Universitaires Notre-Dame de la Paix (FUNDP), Namur, Belgium.
- **Postdoctoral Fellowship Award**, January 2001, Institute for Physical and Theoretical Chemistry, Technical University of Munich, Munich (Germany).
- **Invited seminar**, November 3, 2000, Institut für Physikalische und Theoretische Chemie, Technische Universität München, Munich, Germany.
- **Postdoctoral Fellowship Award**, April 2000, Laboratory of Organic Chemistry, Wageningen University, Wageningen (The Netherlands).
- **Postdoctoral Fellowship Award**, March 1999, Institute for Fundamental Chemistry [presently: Fukui Institute for Fundamental Chemistry, Kyoto University], Kyoto (Japan).
- **Invited seminar**, March 3, 1999, Chemistry and Physics Departments, University of Sfax, Sfax, Tunisia.
- **Invited seminar**, November 24, 1998, Laboratoire de Chimie de Coordination, Toulouse, France.
- **PhD scholarship** from Ministry of Higher Education and Scientific Research of Tunisia for the year 1997/1998.

OTHER ACADEMIC ACTIVITIES AND ACHIEVEMENTS

- Designed and built a **custom-configured supercomputer**, which executes quantum chemistry calculations in parallel, allowing many users to access and submit calculations at the same time.
- Wrote and persuasively presented proposals to executive research teams.

Collaborations:

- **2003–2009** with the distinguished Japanese scientist: Professor R. Noyori (Nobel Prize in Chemistry 2001, Nagoya University).
- **2003–2009** with eminent Japanese scientists in their fields: Professor Y. Takeuchi (Organic Chemistry, Toyama University), Professor K. Kabuto (Organic Chemistry, Tohoku University).
- **2005** with Dr. J. G. Highfield from ICES (Institute of Chemical & Engineering Sciences, Singapore) on theoretical design of novel quasicrystals and their eventual elaboration.
- **2005** with Dr. David Foo from Johnson & Johnson-Singapore on the investigation of the physicochemical properties of melanin.
- **2005** with Rolls-Royce Company (Singapore).
- **2003/01–2005/02** with Professor S. Koseki from (Theoretical Chemistry, co-author of GAMESS quantum chemistry software, Osaka Prefecture University).
- **2001** with the experimental group of Professor J. Libuda (Fritz Haber Institute, Germany).
- **2000** with AkzoNobel company (The Netherlands) with which we had regular meeting on designing innovative materials.

- **1995/12–1998/9** with the materials science group headed by Dr. C. Vahlas (INPT-ENSCT, Toulouse, France) on metal-arene and metallocene compounds.

Others:

- **2005/12/08** invited Professor Nagao Kobayashi from Tohoku University to give seminar in IHPC, Singapore.
- **1999** helped in organizing an international conference on polymers which was held in France.
- Actively interacted with all researchers and students of all the host research groups I have joined.
- Participated to most of the group seminars and discussions.
- Wrote research projects and research reports.
- Helped students in writing their PhD theses and papers.

Languages:

- English: fluent (read, write, speak).
- French: fluent (read, write, speak).

CONTACT DETAILS OF REFEREES

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