CURRICULUM VITAE

Dr. Roger Rousseau

July 13, 2007

1 PERSONAL DATA

Name: Roger Rousseau
Nationality: Canadian
Country of Birth: Canada
Present Address: Pacific Northwest National Laboratory
Richland, Washington 99354, USA **e-mail:** roger.rousseau@pnl.gov

2 ACADEMIC BACKGROUND

University Degrees:
Honors Bachelors of Science (H. B. Sc.), Chemistry, University of Windsor, Windsor, Canada, Sept. 1987–April 1991.
Masters of Science (M. Sc.), Inorganic Chemistry, The University of Michigan, Ann Arbor, USA, Sept. 1991–April 1994 (without thesis).

Doctorate:
Doctor of Philosophy (Ph. D.), Inorganic Chemistry, The University of Michigan, Ann Arbor, Michigan, USA, Sept. 21, 1995.
Thesis Adviser: Professor Stephen Lee
Title of Thesis: "Molecular Orbital Models For Electronic and Structural Properties of Organic and Inorganic Materials"
Detached Study from Ph. D. Program:
Location: Institut de Ciència de Materials de Barcelona (CSIC), Bellaterra, Spain, Oct. 1994–July 1995, with Prof. Enric Canadell

3 PROFESSIONAL EXPERIENCE

3.1 Research

1. Staff Scientist, Pacific Northwest National Lab, Richland, Washington, USA. May 2007-present.
Description of Research: Computational Catalysis.
1. Visiting Associate Professor, Condensed Matter Physics. International School for Advanced Studies, Triesta, Italy. (Concurrent with status as long term visiting scientists at International Center for Theoretical Physics, Trieste, Italy.) March 2003–April 2007.
Description of Research: Large scale computer simulations of surface reactions related to nanotechnology and environmental processes.
2. Research Associate: Lehrstuhl für Theoretische Chemie Ruhr-Universität Bochum, Bochum, Germany, Oct. 2001–Feb 2003.
Description of Research: Large scale computer simulations of biological and nanoscale materials.
3. Theory group–Steacie Institute for Molecular Science, National Research

Council of Canada, Ottawa, Canada, Jam. 1999–Sept 2001,
Description of Research: Computational electronic structure and transport, molecular dynamics and chemical reactivity of solids, surfaces and nanostructures. Construction and administration of PC based cluster for parallel computing.
4. Post Doctoral Research Fellow: Theory group–Steacie Institute for Molecular Science, National Research Council of Canada, Ottawa, Canada, Feb. 1998–Dec. 1998, with Dr. John Tse.
Description of Research: Computational electronic structure and transport, molecular dynamics and chemical reactivity of solids, surfaces and nanostructures.
5. Post Doctoral Research Fellow: Max–Planck–Institut für Festkörperforschung, Stuttgart, Germany, June 1996–Feb. 1998, with Prof. Michele Parrinello
Description of Research: Application of *ab initio* molecular dynamics methods to molecular and solid state systems.
6. Research Assistant, University of Windsor, Canada, May–July 1991, with Prof. Ricardo Aroca.
Description of Research: Electronic Structure calculations of metallated phthalocyanine complexes.
7. Undergraduate Research Assistant: University of Windsor, Canada, May–Aug. 1990, with Prof. Douglas W. Stephan.
Description of Research: Electronic structure calculations of organometallic complexes of titanium and zirconium.

3.2 Teaching

1. Visiting Associate Professor, Condensed Matter Physics. International School for Advanced Studies, Triesta, Italy.
Description of Teaching: Presentation of lectures on quantum chemical electronic structure methods for Condensed Matter and Biological Physics (March-April 2003).
Presentation of lectures and laboratory on Computers in Physics for for Condensed Matter and Biological Physics. (Feb-March 2005, March 2006, March 2007).
2. Teaching Assistant, Dept. of Chemistry, The University of Michigan, USA, Sept. 1991–April 1993.
Description: Preparation of tutorial classes in general chemistry (Sept. 1991–April 1992), organic chemistry (Sept. 1992–Dec. 1992) and inorganic chemistry (Jan. 1993–April 1993).

4 SCHOLARSHIPS AND HONORS

1. Italian Ministry of Education, Visiting Associate Professorship (2003-2007), location of tenure: Condensed Matter Simulations Group, International School

For Advanced Studies, Trieste, Italy.
2. Natural Sciences and Engineering Research Council of Canada, Visiting Fellowship in Canadian Government Laboratory, Feb. 1998–Dec. 1998.
3. Natural Sciences and Engineering Research Council of Canada, Post Doctoral Fellowship, June 1996–Feb. 1998.
4. Natural Sciences and Engineering Research Council of Canada, Post Graduate Scholarship, Sept. 1993–Aug. 1995.
5. Horace H. Rackham School of Graduate Studies of The University of Michigan, Pre-Doctoral Fellow, Sept. 1994–June 1995.
6. The Dept. of Chemistry of The University of Michigan, Dow-Amaco Fellow, Sept. 1993–April 1994.
7. The Dept. of Chemistry of The University of Michigan, Moses Gonberg Fellow, April. 1992–June 1992.
8. Natural Sciences and Engineering Research Council of Canada, Post Graduate Scholarship, April 1991, (Declined: funds not transferable to US universities).
9. Dept. of Chemistry and Biochemistry of the University of Windsor, C. S. Lin Memorial Scholarship, 1991.
10. Society of Chemical Industry Canadian Section, Merit Award for Academic Excellence, 1991.
11. University of Windsor, Medal of Honour for Academic Excellence in Chemistry and Biochemistry, 1991.
12. Canadian Society for Chemistry, Medal for Academic Excellence, 1990.
13. Natural Sciences and Engineering Research Council of Canada, Undergraduate Research Fellowship, 1990.

5 Academic Memberships and Services

5.1 Memberships

1. Member of American Chemical Society (ACS) (1993-present)
2. Member of Italian National Institute for the Physics of Materials (INFM) (2003-2007)
3. Member of Democritos (INFM) (2004-2007)

5.2 Seminar Series and Workshops

1. Director and Co-organizer of ICTP School for "Tools of Computational Physics". ICTP, March 2006.
2. Director and Co-organizer of ICTP Workshop "Advanced School for High Performance Computing Tools for e-science". ICTP, March 2007.
3. Co-organizer of Tutorial on Car-Parrinello Simulations for Biological Systems, Research Science Park, University of Barcelona, Barcelona, Spain, Nov. 2004.
4. Co-organizer of The ICTP/Democritus Informal Chemical Physics Seminar Series, Trieste, Italy. (2003-present).

5. Organizer of Theoretical and Computational Group Seminar Series, Stacie Institute for Molecular Sciences, NRC Canada. (1999-2001).

5.3 Scientific Computing

1. Constructed: 34 processor Pentium III/Dolphin cluster, SIMS, NRC Canada (2001).
2. Advised on Purchase of: 180 processor Athlon/Dolphin cluster Bochum, Germany (2002).
3. Constructed: 280 processor Operon/Myrinet cluster, SISSA, Trieste, Italy (2004-2005).

6 GRANTS

(Funds quoted in USD at exchange rate at time of awarding of grant)

1. Grant type: ICTP School
Issued by: International Center for Theoretical Physics, Trieste Italy (UNESCO).
Grant title: Advanced School on High Performance Computing Tools for e-Science.
Grant amount: $60,000 for course infrastructure
PI: Roger Rousseau, Stefano Cozzini, Axel Kohlmeyer

2. Grant type: ICTP Workshop
Issued by: International Center for Theoretical Physics, Trieste Italy (UNSECO).
Grant title: Course on Tools for Computational Physics.
Grant amount: $30,000 for course infrastructure
PI: Roger Rousseau, Stefano Cozzini, Axel Kohlmeyer

3. Grant type: COFIN 2003 Issued by: Italian Ministry of Research and University (MIUR) Grant title: Electronic and structural properties of weakly bound films Grant amount: approx. $150,000 for investigators at SISSA PI: Erio Tosatti, co-PIs:Sandro Scandolo, Roger Rousseau, Giacinto Scoles

4. Grant type: Visiting Associate Professorship research funds, Issued by: Italian Ministry of Education, Grant amount: $45 000 (US). PI: Roger Rousseau

5. Grant type: Journal Author Grant, Grant Number 01 03 314, Issued by: Royal Society, Grant amount: $2000 (USD), Grant title: Electronic Structure of Polyynl Based Molecular Wires, Grant amount: $2000 (USD) PI: R. Rousseau, co-PI: Dr. P. J. Low (U. Durham), June 2001.

7 PUBLICATIONS

The number of citations of each article is given as compiled by the ISI web of science (date May. 2007) total: 1186 citations, 74 publications.

7.1 Book Chapters and Reviews

1. R. Rousseau and S. Lee in *Graph Theoretical Approaches to Chemical Reactivity*, D. Bonchev and O. Mekenyson (Eds.), Klewer, The Netherlands, (1994), 73–109. Topological control of Molecular Orbital Theory: A Comparison of μ_2–Scaled Húckel Theory and Restricted Hartree–Fock Theory for Boranes and Carboranes.
(citations: 3)

2. J. S. Tse and R. Rousseau in *Computational Molecular Spectroscopy*, P. Bunker and P. Jenson (Eds.), Wiley, New York, (2000) 625-656. Ab Initio Molecular Dynamics.
(citations: 2)

3. R. Rousseau, M. Gener and E. Canadell, *Advanced Functional Materials, (Feature Article)*, **14**, 201–214 (2004). Step-by-Step Construction of the Electronic Structure of Molecular Conductors: Conceptual Aspects and Applications.
(citations: 6)

4. S. Scandolo and R. Rousseau, *Encyclopedia of Condensed Matter Physics)*, F. Bassini, J. Liedl and P. Wyder (Eds.), Elsevier, The Netherlands, 2005. Car-Parrinello Molecular Dynamics.
(citations: 0)

7.2 Letters and Communications

5. A. J. Ashe III, J. W. Kampf, W. Klein and R. Rousseau, *Angew. Chem. Int. Ed. Eng.* **32**, 1065–1066, (1993): German *Angew. Chem.* **103**, 1112–1113, (1993). Structural Evidence of the Aromaticity of Borepins: A comparison of 1–Chloroborepin and Tricarbonyl(1–chloroborepin)molybdenum.
(citations: 10)

6. R. Rousseau, S. Lee, E. Canadell, F. Texidor, C. Viñas and B. Štíbir, *N. J. Chem.* **20**, 277-281, (1996). Proposed Mechanism for the Isomerization of the First Parent Tricarbollide, [nido–7,6,8–$C_3B_7H_{11}$]$^-$, to [nido–7,8,10–$C_3B_7H_{11}$]$^-$.
(citations: 13)

7. C. Rovira, J. Veciana, E. Ribera, J. Tarrés, E. Canadell, R. Rousseau, M. Mas, E. Molins, M. Almeida, R. T. Hemriques, J. Morgado, J.–P. Schoeffel and

J.–P. Pouget, *Angew. Chem. Int. Ed. Eng.* **36**, 2332–2336 (1997). An Organic Spin–ladder Molecular Material.
(citations: 38)

8. R. Rousseau and D. Marx, *Phys. Rev. Lett.* **80**, 2574–2578 (1998). Fluctuations and Bonding in Lithium Clusters.
(citations: 19)

9. R. Rousseau, G. Dietrich, S. Krückeberg, K. Lützenkirchen, D. Marx, L. Schweikhard, and C. Walther, *Chem. Phys. Lett.* **295**, 41–47 (1998). Probing Cluster Dimensionality with Sensor Molecules: Methanol Adsorbed Onto Gold Clusters.
(citations: 28)

10. J. S. Tse, G. Frapper, A. Ker, R. Rousseau and D. D. Klug, *Phys. Rev. Lett.* **82**, 4472–4475 (1999). The Phase Stability and Electronic Structure of K-Ag Intermetallics at High Pressure.
(citations: 7)

11. R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura, *Phys. Rev. Lett.*, **83**, 2218–2221 (1999). Static Structure and Dynamic Correlations in High Pressure H_2S.
(citations: 8)

12. J. S. Tse, K. Uehara, R. Rousseau, A. Ker, C. I. Ratcliffe M. A. White and G. Mackay, *Phys. Rev. Lett.*, **85**, 114-117 (2000). Structural Principles, and Amorphous-like Thermal Conductivity of Na-doped Si- Clathrates.
errata Phys. Rev. Lett., **86**, 4980 (2001).
(citations: 54)

13. R. Rousseau, M. Boero, M. Bernasconi, M. Parrinello and K. Terakura, *Phys. Rev. Lett.*, **85**, 1254–1257 (2000). Ab-initio simulation of phase transitions and dissociation of H_2S at high pressure.
(citations: 8)

14. S. Alavi, R. Rousseau, S.N. Patitsas, G. P. Lopinski, R. A. Wolkow and T. Seideman, *Phys. Rev. Lett.*, **85**, 5372–5375 (2000). Inducing Desorption of Organic Molecules with a Scanning Tunneling Microscope. Theory and Experiments.
(citations: 45)

15. D. Krüger, H. Fuchs, R. Rousseau, D. Marx, and M. Parrinello, *Phys. Rev. Lett.*, **89**, 186402/1–4 (2002). Pulling Monoatomic Gold Wires with Single Molecules – An *Ab Initio* Simulation.
(citations: 41)

16. D. Krüger, R. Rousseau, H. Fuchs, D. Marx, *Angew. Chem. Int. Ed.*

Eng. **42**, 2251–2253 (2003). Towards "Mechano–Chemistry": Mechanically Induced Isomerizations of Supported Gold Clusters. (work highlighted as "hot paper" on web site and on cover of issue).
(citations: 12)

17. E. Schreiner, C. Nicolini, B. Ludolph, R. Ravindra, N. Otte, A. Kohlmeyer, R. Rousseau, R. Winter and D. Marx *Phys. Rev. Lett.*, **92**, 148101 (2004). Folding and Unfolding of an Elastin–Like Oligopeptide: "Inverse Temperature Transition", Re–entrance, and Hydrogen–Bond Dynamics.
(citations: 8)

18. F. Della Sala, R. Rousseau, A. Görling, and D. Marx *Phys. Rev. Lett.*, **92**, 183401 (2004). Quantum and Thermal Fluctuation Effects on Photoabsorption Spectra of Clusters
(citations: 2)

19. R. Rousseau V. Kleinschmidt, U. W. Schmitt and D. Marx *Angew. Chem. Int. Ed. Eng.*, **43**, 4804–4807 (2004). Assigning protonation patterns in water networks in bacteriorhodopsin based on computed IR spectroscopy
(citations: 20)

20. V. De Renzi, R. Rousseau, D. Marchetto, R. Biagi, S. Scandolo and U. del Pennino *Phys. Rev. Lett.*, **95**, 046804 (2005). Metal work function changes induced by organic adsorbates: a combined experimental and theoretical study.
(citations: 23)

21. M. Konôpka, R. Rousseau, I. Štich and D. Marx *Phys. Rev. Lett.*, **95**, 096102 (2005). Electronic Origin of Disorder and Diffusion at a Molecule/Metal Interface: Self–Assembled Monolayers of CH_3S on Cu(111)
(citations: 7)

22. R. Rousseau, K. Uehara, D. D. Klug, J. S. Tse *ChemPhysChem*, **6**, 1703-1706 (2005). Phase Stability and Broken Symmetry Transition of Elemental Lithium up to 140 GPa. (citations: 2)

23. F. Tassone, G.L. Chiarotti, R. Rousseau S. Scandolo, E. Tosatti, *ChemPhysChem*, **6**, 1752-1756 (2005. Dimerization of CO_2 at high pressure and temperature.
(citations: 2)

24. R. Rousseau, R. Mazzarello, and S. Scandolo, *ChemPhysChem*, **6**, 1756-1760 (2005). An Effective Pseudo-Potential for Modeling Thick Gold Surface Slabs for *Ab Initio* Simulations.
(citations: 2)

25. R. Mazzarello, A. Cossaro, A. Verdini, R. Rousseau, L. Casalis, M. F. Danisman, L. Floreano. S. Scandolo, A. Morgante, and G. Scoles, *Phys. Rev. Lett.*,

98, 016102 (2007). Resolving the Structure of a CH_3S Monolayer on Au(111) by the Interplay Between Molecular Dynamics Calculations and Diffraction Measurements.
(citations: 0)

7.3 Full Research Articles

26. D. G. Dick, R. Rousseau, and D. W. Stephan, *Can. J. Chem.* **69**, 357–362 (1991). Lewis Acidic Titanium Species–The Synthesis, Structure, Bonding and Molecular Modeling Considerations of the Complexes $Ti((NMe_2)_3Cl$ and $Ti(NEt_2)_3Cl$.
(citations: 14)

27. J.–C. Zheng, R. Rousseau and S. Wang, *Inorg. Chem.* **31**, 106–110 (1992). Homonuclear Copper Complexes with Multidentate Amino Ligands. Synthesis and Characterization of a Dicopper Zwiterion, Cu_2(1,3–bis(dimethylamino)–2–propanol)$_2Cl_4$ and a Tricopper Compound, Cu_3(1,3–bis(dimethylamino)–2–propanolato)$_2Cl_4$.
(citations: 21)

28. S. Lee, R. Rousseau and C. Wells, *Phys. Rev. B* **46**, 12121–12131 (1992). Optimization of the Main–Group and Late–Transition–Metal Elemental Structures: Gallium, Boron, Zinc, Cadmium and Manganese.
(citations: 20)

29. A. J. Ashe III, W. Klien, and R. Rousseau, *Organometallics* **12**, 3225–3231 (1993). Evaluation of the Aromaticity of Borepin: Synthesis and Properties of 1–Substituted Borepins.
(citations: 11)

30. A. J. Ashe III, W. Klien, and R. Rousseau, *J. Organomet. Chem.* **468**, 21–23 (1994). An Evaluation of the Rotation Barrier About the B-N Bond of 1–Aminoborepins.
(citations: 5)

31. R. Rousseau, A. Orzarowski, R. Aroca, L. O. Soares, and M. Trisc, *J. Mol. Structure* **317**, 287–297 (1994). The Electronic Structure of Metallated Phthalocyanine-NO_2 Adducts.
(citations: 10)

32. J. W. Ho, R. Rousseau and D. W. Stephan, *Organometallics* **13**, 1918–1926 (1994). Synthesis, Structure and Bonding in Zirconium Phosphide (PHR^-), Phosphinidene ($PR_2{}^-$) and Phosphido ($P_3{}^-$) Derivatives. Errata *Organometallics* **14**, 4030 (1995).
(citations: 33)

33. A. J. Ashe III, J. Kampf, S. Pilotek and R. Rousseau, *Organometallics* **13**, 4067–4061 (1994). Secondary Bonding in Organopniciogen Compounds, Comparison of the Structures of Octamethyl–1,1'–distibaferrocene and Octamethyl–1,1'–diarsaferrocene.
(citations: 26)

34. R. Rousseau and S. Lee, *J. Chem. Phys.* **101**, 10753–10765 (1994). Comparison of μ_2–Scaled Hückel Theory and Hartree–Fock Theory of Boranes and Carboranes.
(citations: 8)

35. L. Chen, S. Breeze, R. Rousseau, S. Wang and L. K. Thompson, *Inorg. Chem.* **34**, 454–465 (1995). Polynuclear Copper–Lanthanide Complexes with Amino Ligands. Synthesis, Structure and Spectroscopic Studies of
$Cu^{II}(bdmmp)_2H_2O$, $Pr^{III}Cu^{II}(bdmmpH)(\mu\text{–}OH)(bfacac)_3$,
$[La^{III}Cu^{II}(bdmmp)(bdmmpH)(\mu\text{–}OH)(O_2CCF_3)_3]_2$
and $Cu^{II}{}_4(bdmmp)_2(\mu_4\text{–}O)(O_2CCF_3)_4$,
(bdmmpH=2,6–Bis((diethylamino)methyl)–4–methylphenol;
hfacac=Hexafluoroacetylacetonato).
(citations: 51)

36. R. Rousseau, R. Aroca and M.–L. Rodriguez–Méndez, *J. Mol. Structure* **356**, 49–64 (1995). Extended Hückel Molecular Orbital Model For Lanthanide Bisphthalocyanine Complexes.
(citations: 22)

37. P. Auban–Senzier, A. Audouard, V. N. Laukhin, R. Rousseau, E. Canadell, L. Brossard, D. Jérome and N. D. Kushch. *J. Phys. I France* **5**, 1301–1310 (1995). Magnetoresistance Studies in the Low–Dimensional Organic Metal α–$(ET)_2TlHg((SeCN)_4$ Under Pressure: Experiments and Simulation By Tight Binding Band Structure Calculations.
(citations: 14)

38. L. A. Kushch, V. V. Gritsenko, L. I. Buravov, A. G. Khomenko, G. V. Shilov, O. A. Dyachenko, V. A. Merzhanov, E. B. Yagubskii, R. Rousseau and E. Canadell, *J. Mater. Chem.* **5**, 1633–1638 (1995). The $M(DDDt)_2$ Family of Conducting Complexes: $[Ni(DDDt)_2]_3(AuBr_2)_2$ The First Quasi–Two–Dimensional Metal Stable Down to at Least 1.3 K.
(citations: 17)

39. R. Rousseau, M. R. Palacín, P. Gómez–Romero and E. Canadell, *Inorg. Chem.* **35**, 1179–1184 (1996). Electronic Structure of Layered Oxides Containing M_2O_7 (M=V, Nb) Double Octahedral Slabs.
(citations: 9)

40. R. Rousseau, M.–L. Doublet, E. Canadell, R. P. Shibaeva, S. S. Khasanov, L. P. Rozenberg, N. D. Kushch and E. B. Yagubskii, *J. Phys. I France* **6**, 1527–1554 (1996). Electronic Structure of the α-(BEDT–TTF)$_2$MHg(XCN)$_4$ (M=Tl, K, NH$_4$; X=S, Se) and Related Phases. Synthesis and Crystal Structure of the New Stable Organic Metal α–(BEDT–TTF)$_2$TlHg(Se$_{1-x}$S$_x$CN)$_4$ (x=0.125).
(citations: 35)

41. M. Tillard–Charbonnel, A. Chahine, C. Belin, R. Rousseau and E. Canadell, *Chem. Eur. J.* **3**, 799-805. (1997). Structure and Chemical Bonding in K$_{14}$Cd$_9$Tl$_{21}$, a Compound Containing Both Isolated Tl$_{11}{}^{7-}$ clusters and $^2_\infty$[Cd$_9$Tl$_{10}{}^{7-}$] sheets.
(citations: 6)

42. R. Rousseau and D. Marx, *Phys. Rev. A* **56**, 617-628 (1997). /em Ab Initio Calculations on Small Clusters of Lithium.
(citations: 23)

43. R. Rousseau, E. Canadell, P. Allemany, D. H. Galván, and R. Hoffmann, *Inorg. Chem.* **36**, 4627-4632 (1997). Concerning the origin of the Metal–to–Insulator Transition in H$_{0.33}$MoO$_3$.
(citations: 16)

44. R. Rousseau, A. Figueras and E. Canadell, *J. Mol. Struct. TheoChem.* **424**, 135–143 (1998). Electronic Structure of the α-(BEDT–TTF)$_2$MHg(XCN)$_4$ (M=Tl, K, NH$_4$; X=S, Se) Molecular Metals: On the 1D vs. 2D Character of the Charge Carriers.
(citations: 0)

45. S. S. Khasanov, B. Zh. Narymbetov, L. V. Zorina, L. P. Rozenberg, R. P. Shibaeva, N. D. Kushch, E. B. Yagubskii, R. Rousseau and E. Canadell, *Eur. Phys. J. B* **1**, 419–428 (1998). Concerning the first–order transition in the low–dimensional organic superconductor (BEDO–TTF)$_2$ReO$_4$· H$_2$O. Crystal and electronic band structure below the phase transition (T=170K).
(citations: 12)

46. F. Boucher and R. Rousseau, *Inorg. Chem.* **37**, 2351–2357 (1998). Bonding and electronic properties of Cs$_3$Te$_{22}$.
(citations: 29)

47. E. Ribera, C. Rovira, J. Veciana, J. Tarrés, E. Canadell, R. Rousseau, E. Molins, M. Mas, J.–P. Schoeffel and J.–P. Pouget, J. Morgado, V. Gama, R. T. Hemriques and M. Almeida, *Chem. Eur. J* **5**, 2025-2039 (1999). The (DT-TTF)$_2$M(mnt)$_2$ family of charge transfer salts: From a spin ladder to delocalized conduction electrons interacting with localized magnetic moments.
(citations: 42)

48. R. Rousseau and D. Marx, *J. Chem. Phys.*, **111**, 5091-5101 (1999). The Role of Quantum and Thermal Fluctuations Upon Properties of Lithium Clusters.
(citations: 15)

49. P. J. Low, R. Rousseau, P. Lam, K. A. Udachin, G. D. Enright, J. S. Tse, D. D. M. Wayner and A. J. Carty, *Organometallics*,**18**, 3885–3897 (1999). Polycarbon Ligand Chemistry: Electronic Interaction Between Ruthenium Fragment and a Cobalt Carbon Cluster Core.
(citations: 31)

50. R. Rousseau and D. Marx, *J. Chem. Phys.*, **112**, 761–769 (2000). The Interaction of Gold Clusters and Methanol Molecules: *Ab Initio* Molecular Dynamics of $Au_n^+CH_3OH$ and Au_nCH_3OH.
(citations: 22)

51. R. Rousseau and D. Marx, *Chem. Eur. J.*, **6**, 2982–2993 (2000). Exploring the Electronic Structure of Elemental Lithium: From Small Molecules to Nanoclusters, Bulk Metal, and Surfaces. Cover page *Chem. Eur. J.*, **6**, 3086 (2000)
(citations: 25)

52. S. Alavi, R. Rousseau and T. Seideman, *J. Chem. Phys.* **113**, 4412–4423 (2000). Toward Control of Surface Reactions With a Scanning Tunneling Microscope. Structure and Dynamics of Benzene Desorption from a Silicon Surface.
(citations: 26)

53. L. V. Zorina, S. A. Khasanov, R. P. Shibaeva, M. Gener, R. Rousseau, E. Canadell, L. A. Kushch, E. B. Yagubskii, O. O. Drozdova and K. Yakushi. *J. Mater. Chem.* **10** 2017–2023 (2000). A New Stable Organic Based Metal Based on the BEDO–TTF Donor and the Doubly Charged Nitroprusside Anion, $(BEDO–TTF)_4(Fe(CN)_5NO)$.
(citations: 30)

54. T. J. Snaith, P. J. Low, R. Rousseau, H. Puschmann and J. A. K. Howard, *Dalton Trans.* issue 3, 292-299 (2001). Further Studies of Electronic Interactions Between Metal Fragments Mediated by Ynyl Based Bridging Ligands.
(citations: 11)

55. D. D. Klug, R. Rousseau, Marco Bernasconi, K. Uehara, Y. Le Page and J. S. Tse, *Phys. Rev. B.*, **63**. 104106-1–104106-5 (2001). *Ab Initio* Molecular Dynamics Study of Successive Pressure Induced Phase Transformations in Cristobalite.
(citations: 7)

56. E. Todorov, M. Evans, S. Lee and R. Rousseau, *Chem. Eur. J.*. **7**. 2652–2662 (2001). Energy Isosbestic Points in Third Row Transition Metal Alloys.
(citations: 3)

57. D. Krüger, H. Fuchs, R. Rousseau, D. Marx, and M. Parrinello, *J. Chem. Phys.* **115**, 4776–4785 (2001). Interaction of Short Chain Alkanethiols and Alkanethiolates with Small Gold Clusters: Adsorption Structure and Energetics.
(citations: 55)

58. O. F. Koentjoro, R. Rousseau and P. J. Low *Organometallics*, **20**, 4502-4509 (2001) Electronic Structure of Ruthenium(II) Polyynyl Complexes.
(citations: 24)

59. G. M. Koretshy, M. B. Knickelbein, R. Rousseau and D. Marx, *J. Phys. Chem. A*, **105** , 11197-11203 (2001). A combined Infrared Photodissociation and Electronic Structure study of Ethanol with Small Gold Clusters.
(citations: 5)

60. R. B. Lyubovskii, S. I. Pesotshii, M. Gener, R. Rousseau, E. Canadell, J. A. A. J. Perenboom, V. I. Nizhankovskii, E. I. Zhilyaena, O. A. Bogdanova, and R. N. Lyubovskaya, *J. Mater. Chem.* **12**, 483-488 (2002). Characterization of the Fermi surface of $(BEDO\text{-}TTF)_5[CsHg(SCN)_4]_2$ by magnetoresistance measurements and tight binding band structure calculations
(citations: 10)

61. A. Ker, E. Todorov, R. Rousseau, K. Uehara, F.-X. Lannuzel and J. S. Tse, *Chem. Eur. J.*. **8**. 2787–2798 (2002). Structure and Phase Stability of Binary Zintl-Phase Compounds: Lithium Group 13 Intermetallics and Metal-Doped Group 14 Clathrate Compounds.
(citations: 4)

62. A. Deluzet, R. Rousseau, A Guilbaud, I. Granger, K. Boubekeur, P. Batail, E. Canadell, P. Auban-Senzier and D. Jérome, *Chem. Eur. J.*. **8**. 3884–3900 (2002). An In-Depth Correlation of the Perturbation of the Organic–Inorganic Interface Topology, Electronic Structure and Transport Properties within an Extended Series of 21 Metallic Pseudopolymorphs, $\beta''(BEDT\text{-}TTF)_4\cdot(guest)\cdot(Re_6Q_6Cl_8)$ (Q=S,Se).
(citations: 19)

63. R. Rousseau, E. Schriener, A. Kohlmeyer, and D.Marx, *Biophys. J.* **86**. 1393–1407 (2004) Temperature Dependent Conformational Transitions and Hydrogen Bond Dynamics of the Elastin-Like Octapeptide GVG(VPGVG): a Molecular Dynamics Study.
(citations: 11)

64. M. Konôpka, R. Rousseau, I. Štich, and D. Marx, *J. Am. Chem. Soc.* **126**, 12103–12111 (2004). Detaching Thiolates from Copper and Gold Clusters: Which Bonds to Break ?
(citations: 19)

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7.4 Notes and Conference Proceedings

68. R. Rousseau and D. W. Stephan, *Organometallics* **10**, 3399–3403 (1991). Bonding and Conformational Aspects of Thiolato–Bridged Early–Late Heterobimetallics.
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69. E. Ribera, C. Rovira, J. Veciana, J. Tarrés, E. Canadell, R. Rousseau, E. Molins, M. Mas, J–P. Schoeffel and J.–P. Pouget, J. Morgado, V. Gama, R. T. Henriques and M. Almeida, *Synth. Metals* **102**, 1743–1746 (1999). The $(DT\text{-}TTF)_2M(mnt)_2$ family of compounds.
(citations: 4)

70. S. S. Khasanov, L. V. Zorina, R. P. Shibaeva, N. D. Kushch, E. B. Yagubskii, R. Rousseau, E. Canadell, Y. Barrens, J. Gaultier, and D. Chasseau, *Synth. Metals* **103**, 1853-1856 (1999) Structural Aspects of the Phase Transition in $(BEDO\text{–}TTF)_2ReO_4\cdot H_2O$.
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71. R. Rousseau and J. S. Tse, *Prog. Theor. Phys. Supp.* **138**, 47–59 (2000). Rationalization of the Structure of Binary Alloys in a Real Space Atomic Level

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72. S. Alavi, R. Rousseau, G. P. Lopinski, R. A. Wolkow and T. Seideman, *Faraday Discussion* **117**, 213-229 (2000). Controlling Organic Reactions on Silicon Surfaces With a Scanning Tunneling Microscope: Theoretical and Experimental Studies of Resonance-Mediated Desorption.
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73. R. B. Lyubovskii, S. I. Pesotskii, M. Gener, R. Rousseau, E. Canadell, A. Auduard, L. Brossard, J. A. A. J. Perenboom, V. I. Nizhankovskii, E. I. Zhilyaeva, O. A. Bagdanova and R. N. Lyubovskaya, in *Molecular Low Dimensional and Nanostructured Materials for Advanced Application* A. Graja, B. R. Bulka, F. Kajzar, Eds., NATO Science Series II: Mathematics, Physics and Chemistry, **59** 191-200, (2002), Magnetic Breakdown and Quantum Interference in Quasi Two-Dimensional Organic Conductors (BEDO-TTF)$_5$(CsHg(SCN)$_4$)$_2$ and (BEDT-TTF)$_8$(Hg$_4$CL$_{12}$(C$_6$H$_5$Cl)$_2$).
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8 INVITED PRESENTATIONS

1. National Research Council Canada, Ottawa, Canada, Oct. 1995,
2. University of Michigan, Ann Arbor, USA, Sept. 1997,
3. University of Windsor, Windsor, Canada, Sept. 1997,
4. National Research Council Canada, Ottawa, Canada, Sept. 1997,
5. Universidad de Barcelona, Barcelona, Spain, Nov. 1997,
6. Institute de Materiaux de Nantes, Nantes, France, Dec. 1997,
7. Wayne State University, Detroit, USA, Dec. 1998,
8. CPMD '99 workshop, Schloβ Ringberg, Germany, Jam. 1999.
9. University of South Carolina, Columbia SC, USA, Dec. 2000.
10. McMaster University, Hamilton, Canada, Jan. 2001.
11. AnorMED, Vancouver, Canada, Jan. 2001.
12. University of British Columbia, Vancouver, Canada, Feb. 2001.
13. University of Durham, Durham UK June. 2001.
14. Institute of Materials Science (CSIC), Barcelona, Spain, June. 2001.
15. Swiss Center for Scientific Computing, Manno, Switzerland, Feb. 2002.
16. Max-Plank-Institute for Biophysical Chemistry, Gü)ttingen, Germany, Feb. 2002.
17. University of Western Ontario, London, Canada, May. 2002.

18. Enviroanalysis 2002, Symposium on Surface Spectroscopy and Nanostructures, Toronto, Canada, May 2002.
19. International Center for Theoretical Physics (ICTP), Trieste, Italy, Nov. 2002.
20. Institute of Materials Science (CSIC), Barcelona, Spain, Dec. 2002.
21. University of Montreal, Montreal, Canada, March. 2004.
22. Research Science Park, University of Barcelona, Barcelona, Spain, Nov. 2004.
23. Tutorial on Car-Parrinello Simulations for Biological Systems, Research Science Park, University of Barcelona, Barcelona, Spain, Nov. 2004.
24. INFM -National Research Center on NanoStructures and BioSystems at Surfaces, Universita' di Modena e Reggio Emilia, Modena, Italy, Sept. 2005.
25. National Research Council Canada, Ottawa, Canada, Oct. 2005.
26. Pacific Northwest National Lab, Richland, Washington, USA, July 2006.
27. Pacific Northwest National Lab, Richland, Washington, USA, Jan. 2007.