

# CURRICULUM VITAE

**Fedor Y. Naumkin**

## GENERAL INFORMATION

**Address:** Faculty of Science  
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## DEGREES

**Ph. D** in Laser Physics (Theoretical), General Physics Institute (Moscow, Russ. Acad. Sci.), 1992

Dissertation: *Electronic states of triatomic excimer molecules and their role in the exciplex laser kinetics*

Supervisors: Prof. S. I. Yakovlenko, Dr V. G. Pevgov

**M. Sc.** I hons. in Physics, Moscow State Engineering Physics Institute, 1987

Thesis: *Analysis of parameters of a special-purpose nuclear reactor*

## EMPLOYMENT HISTORY

07.2009 - present	Associate Professor, Faculty of Science, Univ. of Ontario Inst. of Technology The post includes research (40%), teaching (40%), and administration (20%)
07.2004 - 07.2009	Assistant Professor, Faculty of Science, Univ. of Ontario Inst. of Technology
07.1998 - 07.2004	Visiting Assistant Professor, Dept. of Chemistry, Univ. of Toronto, Canada
09.1996 - 07.1998	Research Associate, Dept. of Chemistry, Univ. of Waterloo, Canada
Summer 1996	INTAS Visiting Researcher, Dept. of Chemistry, Univ. of Cambridge, UK
06.1995 - 06.1996	MPI Visiting Scientist, Inst. of Theor. Chemistry, Univ. of Stuttgart, Germany
06.1994 - 06.1995	Royal Society Postdoc. Fellow, School of Chemistry, Univ. of Sussex, UK
1992 - 06.1994	Senior Research Associate, General Physics Institute (Russ. Acad. Sci.)
1987 - 1992	Research Associate, General Physics Institute (Russ. Acad. Sci.), Russia

*All above positions are full-time ones*

## PROFESSIONAL AFFILIATIONS AND ACTIVITIES

Membership: American Chemical Society  
Royal Society of Chemistry

Reviewer: Chemical Physics, Chemical Physics Letters,  
Journal of Chemical Physics,  
Physical Chemistry Chemical Physics,  
Molecular Physics,  
Dalton Transactions, New Journal of Chemistry  
Journal of Physical Chemistry, Journal of Physical Chemistry Letters,  
Theochem, Computational and Theoretical Chemistry,  
Theoretical Chemistry Accounts,  
Spectrochimica Acta,  
Journal of Organic Chemistry

## RESEARCH

### CURRENT RESEARCH INTERESTS

My expertise lies in the domains of Theoretical / Computational Chemistry & Chemical Physics, with a particular focus on interdisciplinary Nanoscience (studies of nanometer-sized systems). The objects of interest are generally specified as polyatomic systems (atomic and molecular complexes and clusters, atoms and molecule on surfaces, interfaces at molecular level). Present directions of research focus on core-shell cluster nano-systems with molecular species inside metal-atom cages (interacting non- and covalently), and on intermolecular junctions mediated by ion-pair links or metal atoms. Other interests include multi-electronic-state model potentials, determination and efficient representation of multi-dimensional intermolecular potential surfaces. The main aims are to predict new stable structures and compositions, to investigate relationships between various properties, and ultimately to design systems with desirable characteristics. Potential practical applications of my work include development of new materials with unique properties, novel catalytic agents, elements of molecular electronics and machinery, molecular storage and transport, energy storage at molecular level.

### AWARDS / GRANTS

Source: Canadian Foundation of Innovation (CFI)  
Project: Computational Science and Visualization Laboratory  
Amount: \$12,500 (out of \$100,000 total)  
Investigators: G. Lewis (PI), **F. Naumkin**, and 6 other investigators  
Date awarded: 2005

Source: Discovery Grant (Individual), NSERC  
Project: Design and characterization of hard and soft filled cluster cages  
Amount: \$24,500 / year for 5 years  
Date awarded: April 2007

Source: SHARCnet (academic research computing network)  
Purpose: Undergraduate student research fellowship  
Amount: \$7,000  
Date awarded: June 2007

Source: Royal Society of Chemistry (UK), International Authors Grant  
Purpose: Travel assistance for a collaborative research in the Univ. of Cambridge (UK)  
Amount: £2500  
Date awarded: March 2010

### COLLABORATIONS

**Prof. O. Roncero**, Institute of Fundamental Physics, C.S.I.C., Madrid (Spain)  
Project: Implementation of analytical-derivative algorithm for atomic cluster-ion potential  
(Sabbatical leave at the IFP, C.S.I.C., 2015)

**Prof. D. J. Wales**, University of Cambridge (UK)  
Projects: Development and application of intermolecular potentials for polyatomic systems  
(1-month visit to the Univ. of Cambridge, 06-07.2007);  
Design and property analysis of core-shell molecule@metal-cage cluster systems  
(Sabbatical leave at the Univ. of Cambridge, 2010-11).

**Dr F. Calvo**, University of Lyon (France)  
Project: Molecular dynamics simulation of atomic/molecular ionic clusters with model potentials.

**Prof. J. C. Polanyi**, University of Toronto (Canada)  
Project: Modelling of adsorption and reactions of halo-/organic molecules on solid Si surfaces.

## PUBLICATIONS

**Count:** Total of **2** book chapters and **69** papers (*see the attached Publication List*).

**Citation index** (by the Institute for Scientific Information): **540+** references to published work (no self-)

**h-index:** 16

**Overview:**

- 2 chapters in books
- 11 papers in J. Chem. Phys.
- 7 papers in Chem. Phys. Lett.
- 5 papers in Chem. Phys.
- 2 papers in ChemPhysChem
- 6 papers in Phys. Chem. Chem. Phys.
- 8 papers in Mol. Phys.
- 1 paper in Comput. Phys. Commun.
- 5 papers in J. Phys. Chem. A
- 2 papers in Faraday Discuss.
- 1 paper in New J. Chem.
- 1 paper in Int. J. Quant. Chem.
- 1 paper in Comput. Theor. Chem.
- 3 papers in Surf. Sci.
- 9 papers in Sov. Phys. - Lebedev Inst. Reports / Bulletin of Lebedev Phys. Inst.
- 3 papers in General Physics Institute Proceedings

## PRESENTATIONS

**58 papers presented at meetings and symposia** (in inverse-chronological order)

- 1) **F. Y. Naumkin** and K. Fisher, Metal-organic molecular units with charge-controlled structures. 98<sup>th</sup> CSC meeting, Ottawa, Canada, June 13-17, 2015.
- 2) **F. Y. Naumkin** and D. J. Wales, Encapsulation of atomic hydrogen in metal cluster cages and their assemblies: Towards hydrogen-filled nanofoams. 98<sup>th</sup> CSC meeting, Ottawa, Canada, June 13-17, 2015.
- 3) **F. Y. Naumkin**, Core-shell metallocarbons: Property alteration and structure control. 98<sup>th</sup> CSC meeting, Ottawa, Canada, June 13-17, 2015.
- 4) **F. Y. Naumkin** and D. J. Wales, Towards light-metal nanofoams for hydrogen storage: Trapping hydrogen in assemblies of metal cluster cages. 98<sup>th</sup> CSC meeting, Ottawa, Canada, June 13-17, 2015.
- 5) **F. Y. Naumkin**, Core-shell metallocarbons: Property alteration and charge-controlled structural dynamics, 20<sup>th</sup> MOLEC European Conference, Gothenburg, Sweden, Aug. 2014.
- 6) **F. Y. Naumkin** and K. Fisher, Electronic-perturbation induced structural dynamics of metal-organic molecular sandwiches, 20<sup>th</sup> MOLEC European Conference, Gothenburg, Sweden, Aug. 2014.
- 7) B. J. Irving and **F. Y. Naumkin**, Al-kanes and Al-kenes. 97<sup>th</sup> Canadian Chemistry Conference, Vancouver, Canada, June 2014. (*Talk*)
- 8) **F. Y. Naumkin**, Molecular vs atomic encapsulation of hydrogen in metal cluster-cage assemblies, VIII<sup>th</sup> Congress of the Int. Society of Theor. Chem. Physics, Budapest, Hungary, Aug. 2013. (*Talk*)
- 9) **F. Y. Naumkin**, Metal-organic molecular interfaces: Options for induced structure manipulation. 44<sup>th</sup> IUPAC World Chemistry Congress, Istanbul, Turkey, Aug. 2013. (*Talk*)
- 10) **F. Y. Naumkin** and D. J. Wales, Hydrogen in metal cluster-cage assemblies: molecular vs atomic encapsulation options. 44<sup>th</sup> IUPAC World Chemistry Congress, Istanbul, Turkey, Aug. 2013. (*Talk*)
- 11) **F. Y. Naumkin**, Metal-organic molecular units for induced structure manipulation. 28<sup>th</sup> Symposium of Chemical Physics, Waterloo, Nov. 2012. (*Talk*)
- 12) **F. Y. Naumkin**, D. J. Wales, Hydrogen in light-metal cage assemblies: Towards a nanofoam storage, XVII Int. Workshop on Quant. Systems in Chem. and Phys., Turku, Finland, Aug 2012. (*Invited talk*)
- 13) **F. Y. Naumkin** and D. J. Wales, Hydrogen in light-metal cage assemblies: Towards a nanofoam storage, 4<sup>th</sup> EuCheMS meeting, Prague, Czech Republic, Aug 2012.
- 14) **F. Y. Naumkin** and G. Kocchar, Metal-mediated molecular junctions: a computational design.

- 94<sup>th</sup> Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
- 15) **F. Y. Naumkin**, Shape design and property alterations of aurocarbon core-shell species.  
94<sup>th</sup> Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
  - 16) **F. Y. Naumkin**, Computational exploration of cluster species with molecular cores inside metal-atom shells. 94<sup>th</sup> Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
  - 17) **F. Y. Naumkin** and D. J. Wales, Hydrogen@metal core-shell cluster species: towards efficient in-cage storage. 94<sup>th</sup> Canadian Chem. Conf., Montreal, Canada, June 2011. (*Talk*)
  - 18) **F. Y. Naumkin** and G. Kocchar, Organic molecules linked by metal atoms: sandwich- and trap-type interfaces. 94<sup>th</sup> Canadian Chemistry Conf., Montreal, Canada, June 2011. (*Talk*)
  - 19) **F. Y. Naumkin**, Computational design of metal-mediated molecular junctions.  
3<sup>rd</sup> EuCheMS Congress of Chemistry, Nurnberg, Germany, Aug.-Sep. 2010. (*Talk*)
  - 20) **F. Y. Naumkin** and G. Kocchar, Un/usual coordination of carbon in hyper/metallide CM<sub>n</sub> species. 25<sup>th</sup> Symposium of Chemical Physics, Waterloo, Nov. 2009. (*Talk*)
  - 21) **F. Y. Naumkin** and P. McNelles, Hydrogen in metal cluster cages: weak bonding and reactions in confined spaces.  
238<sup>th</sup> ACS National Meeting, Washington, U.S., August 2009. (*Talk*)
  - 22) G. Kochhar, P. McNelles, **F. Y. Naumkin**, Carbon aurides and hyper-aurides: usual and unusual coordination of carbon.  
238<sup>th</sup> ACS National Meeting, Washington, U.S., August 2009. (*Talk*)
  - 23) **F. Y. Naumkin** and P. McNelles, Hydrogen in metal cluster cages: weak bonding and reactions in confined spaces. 42<sup>nd</sup> IUPAC Congress, Glasgow, UK, August 2009. (*Talk*)
  - 24) G. Kochhar, P. McNelles, **F. Y. Naumkin**, Carbon aurides and hyper-aurides: unusual coordination of carbon and other properties.  
42<sup>nd</sup> IUPAC Congress, Glasgow, UK, August 2009.
  - 25) **F. Y. Naumkin** and P. McNelles, Hydrogen in metal cluster cages: weak bonding and reactions in confined spaces.  
92<sup>nd</sup> Canadian Chemistry Conference, Hamilton, Canada, May-June 2009. (*Talk*)
  - 26) G. Kochhar, P. McNelles, **F. Y. Naumkin**, Carbon aurides and hyper-aurides: unusual hybridization in carbon and other properties.  
92<sup>nd</sup> Canadian Chemistry Conference, Hamilton, Canada, May-June 2009. (*Talk*)
  - 27) **F. Y. Naumkin** and P. McNelles,  
Hydrogen nano-storage in metal clusters: Low-temperature release option.  
ICH2P (Int. Conf. on Hydrogen Production), Oshawa, Canada, May 2009. (*Talk*)
  - 28) **F. Y. Naumkin**, Gold shells shaped by carbon cores: From Au<sub>18</sub> cage to C<sub>10</sub>Au<sub>18</sub> aurocarbon.  
TACC 2008, Shanghai, China, Sept. 2008. (*Invited talk*)
  - 29) **F. Y. Naumkin**, Unusual structural and electronic features of small C<sub>n</sub>Al<sub>m</sub> clusters.  
TACC (Int. Conf. on Theory & Appls. of Comput. Chem.) 2008, Shanghai, China, Sept. 2008.
  - 30) **F. Y. Naumkin**, Dividing the charge and conquering the valence: Novel trapped-molecule complexes with penta-valent carbon.  
23<sup>rd</sup> Symposium on Chemical Physics, November 2007, Waterloo, Canada. (*Talk*)
  - 31) **F. Y. Naumkin**,  
Metal cluster-cages shaped by molecular fillers: Towards flexible design of parameters.  
COMET (Conf. on Molec. Energy Transfer) XX, Arcachon, France, June 2007. (*Talk*)
  - 32) **F. Y. Naumkin**, High-energy intermolecular sandwiches: harpooning through a molecule.  
COMET (Conf. on Molec. Energy Transfer) XX, Arcachon, France, June 2007.
  - 33) **F. Y. Naumkin**,  
Criminal applications of Quantum Mechanics: Putting molecules behind nano-bars.  
Conference on Molecular Quantum Mechanics, Budapest, Hungary, May 2007.
  - 34) **F. Y. Naumkin**, Nano-jewellery: C<sub>5</sub>Au<sub>12</sub> – a gold-plated diamond at molecular level.  
ISSPIC (Int. Symp. on Small Particles & Inorg. Clusters) XIII, Göteborg, Sweden, July 2006.
  - 35) **F. Y. Naumkin** and H. Leung,  
Induced super-halogen behavior of metal moieties in halogen-doped metal clusters.  
APS March Meeting, Baltimore, USA, 2006. (*Talk*)
  - 36) S. Dobrin, K. R. Harikumar, R. V. Jones, **F. Y. Naumkin** and J. C. Polanyi  
First STM investigation of long-chain halo-alkanes adsorbed at the Si(111) surface:

- Reactive and non-reactive interactions between the molecule and the surface.  
NSERC Nano Innovation Platform: Ontario NanoConference, Toronto, Canada, 2004.
- 37) G.-P. Jiang, X. K. Lu, C. Matta, **F. Y. Naumkin**, I. Petsalakis, J. C. Polanyi, H. Rajamma, D. Rogers, G. Theodorakopoulos, and J. Yang, Thermal, photo-induced and electron-induced reaction of adsorbates on Si, followed by STM.  
226 American Chemical Society National Meeting, New York, USA, 2003.
  - 38) S. A. Dobrin, J. B. Giorgi, T. G. Lee, H. He, **F. Y. Naumkin**, J. C. Polanyi, S. A. Raspopov, and J. Wang, Dynamics of photoinduced charge-transfer reactions at surfaces: Hydrogen halides on sodium clusters preadsorbed on LiF(001).  
224 American Chemical Society National Meeting, Boston, USA, 2002.
  - 39) **F. Y. Naumkin**, J. C. Polanyi, and D. Rogers,  
Adsorption of chloro-derivatives of benzene on Si(100)2×1.  
Conference on Exploring Modern Computational Chemistry (EMC<sup>2</sup>), Nottingham, UK, 2002.
  - 40) S. Dobrin, J. B. Giorgi, T. G. Lee, H. He, **F. Y. Naumkin**, J. C. Polanyi, S. A. Raspopov, and J. Wang, Photoinduced charge-transfer reactions between sodium clusters and HF, HCl, HBr adsorbed on LiF.  
International Workshop on Nanochemistry, Vienna, Austria, 2002.
  - 41) S. A. Raspopov, N. S. K. Sze, **F. Y. Naumkin**, J. B. Giorgi, and J. C. Polanyi, Photoinduced dynamics of Cl<sub>3</sub> radical-molecule complex prepared and studied at LiF (001) surface  
223 American Chemical Society National Meeting, Orlando, USA, 2002.
  - 42) A. J. Hudson, **F. Y. Naumkin**, H. B. Oh, J. C. Polanyi, and S. A. Raspopov,  
Dynamics of harpooning studied by transition state spectroscopy: III. LiFCH<sub>3</sub>  
Faraday Discussions 118 (Cluster dynamics), Durham, UK, 2001. (*Talk*)
  - 43) A. J. Hudson, **F. Y. Naumkin**, H. B. Oh, S. A. Raspopov, and J. C. Polanyi  
Dynamics of Harpooning in Li...FCH<sub>3</sub> van der Waals complex  
Gordon Research Conference on Molecular Energy Transfer, Ventura, USA, 2001.
  - 44) J. B. Giorgi, T. G. Lee, A. J. Hudson, **F. Y. Naumkin**, H. B. Oh, P. Piecuch, and J. C. Polanyi  
Harpooning studied by transition state spectroscopy, M...XR + hν → [M\*...XR] → [M<sup>+</sup>...XR<sup>-</sup>]  
→ products: Results for M = Li, X = F, R = CH<sub>3</sub> or H  
219th American Chemical Society National Meeting, San Francisco, USA, 2000.
  - 45) S.A. Raspopov, J.B. Giorgi, T.G. Lee, **F.Y. Naumkin**, J. Wang, and J.C. Polanyi  
Photoinduced charge-transfer reactions of (HCl)<sub>m</sub>...Na<sub>n</sub> complexes on LiF(001) surface: reactive and non-reactive pathways  
Gordon Research Conf. on Atomic and Molecular Interactions, New London, USA, 2000.
  - 46) J. B. Giorgi, T. G. Lee, **F. Y. Naumkin**, J. C. Polanyi, S. A. Raspopov, and J. Wang, Photoinduced charge-transfer reaction at surfaces:  
(HCl)<sub>m</sub>Na<sub>n</sub>/LiF(001) + hν(640 nm) → (HCl)<sub>m-1</sub>ClNa<sub>n</sub>/LiF(001) + H(g)  
Faraday Discussions 117 (Excited states at surfaces), Nottingham, UK, 2000.
  - 47) S. A. Raspopov, N. S.-K. Sze, **F. Y. Naumkin**, J. B. Giorgi, and J. C. Polanyi  
Surface aligned photochemistry: Photodissociation of Cl<sub>2</sub> and Cl<sub>2</sub>...Cl adsorbed on LiF (001)  
Gordon Research Conference on Dynamics at Surfaces, Andover, USA, 1999.
  - 48) J.B. Giorgi, T.G. Lee, A.J. Hudson, **F. Naumkin**, H.-B. Oh, P. Piecuch, and J.C. Polanyi  
Harpooning studied by transition-state spectroscopy:  
M + XR + hν → M\*...XR → M<sup>+</sup>...XR<sup>-</sup> → products (X = F, Cl, Br; R = H, CH<sub>3</sub>)  
Symposium "Electronically Nonadiabatic Processes in Gaseous, Cluster, Condensed Media", 218th American Chemical Society National Meeting, New Orleans, USA, 1999.
  - 49) **F. Y. Naumkin** and F. R. W. McCourt, Predicted microwave spectrum as a simultaneous product of both linear and T-shaped conformers of the ground state He-Cl<sub>2</sub> system.  
53rd OSU Int. Symp. on Molecular Spectroscopy, Columbus, USA, 1998. (*Talk*)
  - 50) **F. Y. Naumkin**, F. R. W. McCourt, and R. J. Le Roy  
On the "hidden" microwave spectrum of the ArCl<sub>2</sub> linear conformer  
52 OSU International Symposium on Molecular Spectroscopy, Columbus, USA, 1997.
  - 51) **F. Y. Naumkin** and F. R. W. McCourt,  
Optical (microwave) spectra of the Van der Waals complexes of Rg atoms with molecules  
Int. Conf. on Optical, Electric & Magnetic Properties of Molecules, Cambridge, UK, 1997.

- 52) **F. Y. Naumkin** and H.-J. Werner, "Triatomics in Molecules" - a method for construction of global potential energy hypersurfaces for molecular clusters  
DFG Colloquium on Molecular Clusters, Pocking, Germany, 1996.
- 53) **F. Y. Naumkin** and P. J. Knowles, Combined empirical - model - *ab initio* potentials for complexes of rare gas atoms with diatomic molecules  
Femtochemistry Conference, Lausanne, Switzerland, 1995.
- 54) **F. Y. Naumkin** and P. J. Knowles, On the adequacy of pairwise additive potentials for rare gas - halogen systems: The effect of anisotropy of interactions between atoms  
XIV Conference on Molecular Energy Transfer, Kloster Banz, Germany, 1995.
- 55) **F. Y. Naumkin** and P. J. Knowles,  
On the adequacy of pairwise additive potentials for dynamical studies of rare gas - halogen systems: The effect of anisotropy of interactions between atoms  
CCP6 Workshop on Intramolecular Dynamics, Oxford, UK, 1994.
- 56) **F. Y. Naumkin**, Electronic spectra of rare gas cluster ions and excimers  
27th Quantum Theory Conference, Sheffield, UK, 1994. (*Talk*)
- 57) **Naumkin F. Y.**, Pevgov V. G. Energy and transition spectra of  $Rg_3^+$  and  $Rg_3^*$  ( $Rg = Ne - Xe$ )  
All-Union Conference on Spectroscopy of gas-discharge laser active media, Lohusalu-Tallinn, USSR, 1990. (*Talk*)
- 58) **Naumkin F. Y.** Electronic structure and optical spectra of rare gas triatomic ions and excimers  
X All-Union Conference on Theory of atoms and atomic spectra, Tomsk, USSR, 1989. (*Talk*)

### Invited lectures and seminars

- **F. Y. Naumkin**, Modelling of unusual core-shell systems: Metallocarbons & metal-cage trapped hydrogen. Chemical Physics Seminar, Inst. Fund. Phys., C.S.I.C., Madrid, Spain, Feb 11, 2015.
- **F. Y. Naumkin**, Trapping, linking and encapsulating molecules in metal-based complexes and cluster cages. Cavendish Lab – ESDG Seminar, University of Cambridge, UK, Dec 1, 2010.
- **F. Y. Naumkin**, Trapping, linking and encapsulating molecules in complexes and cluster cages. Physical Chemistry Seminar, Univ. of Nottingham, UK, Nov 24, 2010.
- **F. Y. Naumkin**, Computationally trapping, linking, attaching and encapsulating molecules in complexes and clusters. Molec. Processes & Theory Seminar, University of Birmingham, UK, Nov 15, 2010.
- **F. Y. Naumkin**, Metal-mediated molecular traps and junctions: a computational design. Theoretical Chemistry Seminar, University of Cambridge, Cambridge, UK, Nov 10, 2010.
- **F. Y. Naumkin**, Computational exploration of new polyatomic systems. Sharcnet-sponsored seminar, Faculty of Science, UOIT, April 2010.
- **F. Y. Naumkin**, Unlikely systems: Molecules trapped in complexes and clusters. Department of Chemistry Seminar, University of Cambridge, Cambridge, UK, July 2007.
- **F. Y. Naumkin**, Core-shell aurocarbons: Golden cages filled with molecular carbon radicals. Chemical Physics Seminar, University of Waterloo, Canada, February 2007.

#### Other seminars:

- 2 Chemical Physics Seminars, University of Waterloo (Canada), 1997, 1998
- School of Chemistry, University of Birmingham (UK), 1996
- 2 Department of Chemistry Seminars, University of Cambridge (UK), 1994, 1996
- 2 - Institute of Theoretical Chemistry, University of Stuttgart (Germany), 1995, 1996
- School of Chemistry and Molecular Sciences, University of Sussex (UK), 1994

## TEACHING

### Courses taught and designed

#### (i) Undergraduate courses:

<i>UOIT:</i>	CHEM 2010U	Structure and Bonding *	(2004 - 14)
	CHEM 3140	Physical Chemistry for Biosciences *	(2007 - 14)
	CHEM 4060	Quantum Chemistry and Spectroscopy *	(2012 - 14)
	CHEM 2040U	Thermodynamics and Kinetics *	(2005 - 09)
	CHEM 3040U	Fundamentals of Physical Chemistry *	(2006)
	PHY 2050U	Thermodynamics and Heat Transfer *	(2005 - 12)
	PHY 4030 U	Modern Physics *	(2007 - 13)
	PHY 3020U	Quantum Mechanics I *	(2005 - 06)
	SCIE 1910U	Science in Context/section (team-taught) <sup>†</sup>	(2004 - 06, 09)

Each course is 1-term and normally involves: course planning, lectures (3 hrs/week) preparation and delivery, tutorial (1 hr/week), office consultations (2 hrs/week), test and exam preparation, conducting and marking, and final grading.

\* major responsibility for the course design

<sup>†</sup> 3hr lecture by each participant

<i>Univ. of Toronto:</i>	Physical Chemistry for Life Sciences *	(1998-2004)
	Chemical Kinetics and Dynamics *	(2002)
	Applications of Quantum Mechanics *	(2000)

#### (ii) Graduate courses (M. Sc.):

<i>UOIT:</i>	MCSC 6170	Computational Chemistry * (within the Modeling & Computational Science program)	
	MTSC 6020	Advanced Topics in Materials Science / Atomic nanoclusters module * (within the Materials Science program)	(2008 - 09)
	MTSC 6010	Physics and Chemistry of Materials Chemistry module (within the Materials Science program)	(2012 - 13)

### Other teaching and lectures given

<i>UOIT courses:</i>	PHY 4020	Quantum Mechanics II (2 lectures)	(2006)
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### Incorporation of IT in teaching

Teaching grad courses to students in another University via the Access Grid facility.

Computer-based lecture materials and assignments, and online marking, e.g. via WebCT, Blackboard.

Use of web-based materials:      - subject-oriented applets and supporting texts,  
   - online databases (NIST Chemistry and Physics ones, etc.)

Examples and problem solving in class and homework, using appropriate software tools such as:

- Maple (solving algebraic and differential equations, integration, making plots, etc.),
- Orbital Viewer (construction and plotting of molecular orbitals),
- ChemBio3D, Spartan (user-friendly interfaced quantum-mechanical calculations),
- etc.

## Student projects supervised

### *B.Sc. students (4<sup>th</sup>-year Theses completed):*

P. McNelles, Nano-encapsulation for storage and controlled release of molecular loads	09.07-04.08
G. Kochhar, Design and property analysis of novel aurocarbon polyatomic species	09.08-04.09
F. Momand, Molecular modeling of hydrogen capture in carbon-based systems	09.09-04.10
B. Cochrane, Molecules in ion-pair traps: prediction of parameters of extreme systems	09.12-04.13

### *Undergraduate students (research projects):*

H. Leung, Computational experiment on metal-nonmetal nano-aggregates ‡	06-08.2005
P. McNelles, Design and characterization of molecule-doped metal clusters ‡	05-08.2006
G. Kochhar, Organic-molecular junctions via ion-pair linkers: comput. design ‡	05-08.2007
P. McNelles, Novel metal-halocarbon molecular systems with pentavalent C atoms ‡	05-08.2008
G. Kochhar, Comput. modelling of mixed metal-nonmetal core-shell nanosystems ‡	05-08.2008
G. Kochhar, Structures, stabilities, and properties of "metallo-benzenes" and their extensions ‡ (Best poster award at the UOIT Student Research Day, Aug. 2009)	05-08.2009
K. Fisher, Computational modeling of metal-mediated intermolecular junctions ‡	05-08.2012
B. Cochrane, Computational studies of systems of ion-pair-trapped molecules	09-12.2013
S. Kerr, Computational evaluation of extended metal-organic complexes	09-12.2014
‡ reported by the students at the Science Faculty and UOIT Student Research Days (Aug. 2005-09,12)	

## Postdoctoral supervision

R. Chelat	Postdoctoral assistant	05.2012 – 11.2012
B. Irving	Postdoctoral assistant	01.2013 – 07.2014



## ***SERVICE AND ADMINISTRATION***

### **University service**

- 2015: Graduate Exam Committee chair, M. Sc. Thesis, J. Cervi, UOIT Fac. Of Science
- 2011 - 14: Undergraduate Program Director of Chemistry
- 2004 - 14: Faculty of Science Council member
- 2005 - 14: Chemistry & Physics Faculty-Appointment and Tenure Committee member
- 2007 - 14: Academic Integrity Committee member, Faculty of Science
- 2007 - 14: Faculty of Science liaison with the UOIT Library
- 2014: External examiner, M.Sc. Thesis, A. Naser, UOIT Fac. of Sci.
- 2004 - 13: Ontario University Fairs, UOIT Faculty of Science representative
- 2013: Organizer of International teaching faculty visit (from Czech Republic)
- 2006 - 10: UOIT Academic Council member
- 2008 - 10: UOIT Open Houses, Faculty of Science representative (March, November)
- 2010: Lecturer at a mini-seminar "Who knew?", Science Rendezvous, UOIT
- 2007 - 09: Graduate Committee member, M.Sc. Thesis, J. Findlay, UOIT Fac. of Science
- 2008 - 09: Chemistry division representative, "Show and Tell" tablet-use meeting
- 2008: External examiner, M.A.Sc. Thesis, Y. Hazeli, UOIT Fac. of Eng. & Appl. Sci.
- 2008: UOIT Faculty of Science participant, Teaching Squares
- 2008: Judge of presentations, UOIT Student Research Day
- 2006 - 08: Participation in the Canada Team visit (project discussion)
- 2004 - 07: Invigilator of midterms/exams for other UOIT Faculty of Science courses
- 2007: Organizing Committee member and "Physical Chemistry" session chair, 35<sup>th</sup> South-Ontario Univ. Student Chemistry Conference (SOUSCC), UOIT

### **Other service activities**

- 2008: Chair of the "Materials and Nano" session, International Conference on Theory and Applications of Computational Chemistry, Shanghai, China
- 2008: SHARCnet proposal-review committee member, Round 8, Programming competition
- 2006: Participation in the Ontario Science Grade 11-12 Curriculum Task Force

## PUBLICATION LIST

**Fedor Y. Naumkin**

### Refereed publications

#### (i) Chapters in books

- 1) **F. Y. Naumkin**, Rational design of mixed nanoclusters: Metal shells supported and shaped by molecular cores. (Invited chapter)  
RSC Theoretical and Computational Chemistry Series No.4, Computational Nanoscience, Ed. E. Bichoutskaia, pp. 26-57 (2011).
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