

PUBLICATION LIST

Fedor Y. Naumkin

Refereed publications

(i) Chapters in books

- 1) **F. Y. Naumkin** and D. J. Wales, Hydrogen in light-metal cage assemblies: Towards a nano-foam storage. In: *Advances in Quantum Methods and Applications in Chemistry, Physics, and Biology*. Eds. M. Hotokka, E. J. Brandas, J. Maruani, G. Delgado-Barrio. *Progress in Theoretical Chemistry and Physics*, Volume 27, pp. 211-220 (2013).
- 2) **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).

(ii) Articles in refereed journals (including accepted for publication)

- 1) **F. Y. Naumkin** and D. J. Wales, Counterion-Trapped-Molecules: From High Polarity and Enriched IR Spectra to Induced Isomerization.
ChemPhysChem 21 (2020) 348-355.
- 2) N. O. Laschuk, A. Obua, I. I. Ebralidze, H. M. Fruehwald, J. Poisson, J. G. Egan, F. Gaspari, **F. Y. Naumkin**, E. B. Easton and O. V. Zenkina
Spacer Conjugation and Surface Support Effects in Monolayer Electrochromic Materials.
ACS Appl. Electron. Mater. 1 (2019) 1705-1717.
- 3) J. G. Egan, A. J. Hynes, H. M. Fruehwald, I. I. Ebralidze, S. D. King, R. A. M. Esfahani, **F. Y. Naumkin**, E. B. Easton and O. V. Zenkina, A novel material for the detection and removal of mercury(II) based on a 2,6-bis(2-thienyl)pyridine receptor.
J. Mater. Chem. C 7 (2019) 10187-10195.
- 4) **F. Naumkin**, P. del Mazo-Sevillano, A. Aguado, Y. V. Suleimanov and O. Roncero,
Zero pressure and high pressure mechanisms in the complex forming reactions of OH with methanol and formaldehyde at low temperatures.
ACS Earth and Space Chem. 3 (2019) 1158-1169.
- 5) N. O. Laschuk, I. I. Ebralidze, J. Poisson, J. G. Egan, S. Quaranta, J. T. Allan, H. Cusden, F. Gaspari, **F. Y. Naumkin**, E. B. Easton and O. V. Zenkina,
Ligand Impact on Monolayer Electrochromic Materials Properties.
ACS Applied Materials & Interfaces 10 (2018) 35334-35343.
- 6) S. Kerr and **F. Y. Naumkin**, Noncovalently bound complexes of polar molecules: Dipole-inside-of-dipole vs dipole-dipole systems.
New J. Chem. 41 (2017) 13576-13584.
- 7) **F. Y. Naumkin**,
Dipoles inside of dipoles: Insertion complexes of polar vs nonpolar molecules in ion-pairs.
J. Phys. Chem. A 121 (2017) 4545-4551.
- 8) **F. Y. Naumkin** and D. J. Wales,
Trapping of hydrogen atoms inside small beryllium clusters and their ions.
Chem. Phys. Lett. 659 (2016) 282-288.
- 9) B. Cochrane and **F. Y. Naumkin**, Reshaping and linking of molecules in ion-pair traps.
Chem. Phys. Lett. 643 (2016) 137-141.

- 10) C. Sanz-Sanz, A. Aguado, O. Roncero and **F. Naumkin**,
Non-adiabatic couplings and dynamics in proton transfer reactions of H_n^+ systems:
Application to $H_2 + H_2^+ \rightarrow H + H_3^+$ collisions.
J. Chem. Phys. 143 (2015) 234303.
- 11) B. J. Irving and **F. Y. Naumkin**, A computational cogitation of $C_n@Al_{12}$ clusters,
ChemPhysChem 16 (2015) 233-242.
- 12) B. J. Irving and **F. Y. Naumkin**, A density functional investigation of structure-property
evolution in the tetrakis hexahedral C_4Al_{14} nanocluster,
J. Chem. Phys. 141 (2014) 131102.
- 13) B. J. Irving and **F. Y. Naumkin**, A computational study of 'Al-kanes' and 'Al-kenes',
Phys. Chem. Chem. Phys. 16 (2014) 7697-7709.
- 14) **F. Y. Naumkin** and K. Fisher,
Small metal–organic molecular sandwiches: Versatile units for induced structure manipulation.
Chem. Phys. Lett. 590 (2013) 52-57.
- 15) **F. Y. Naumkin**,
Shape and property alteration of small silver clusters via doping by carbon: CAg_n ($n \leq 6$)
Comput. Theor. Chem. 1021 (2013) 191-196. (Invited paper for a Special Issue.)
- 16) C. N. Ramachandran and **F. Y. Naumkin**,
Structure and properties of small aurocarbons: A selective study.
J. Phys. Chem. A 117 (2013) 6803-6808.
- 17) F. Calvo, **F. Y. Naumkin**, and D. J. Wales,
Nuclear quantum effects on the stability of cationic neon clusters.
Chem. Phys. Lett. 551 (2012) 38-41.
- 18) **F. Y. Naumkin** and D. J. Wales,
Hydrogen trapped in Be_n cluster cages: The atomic encapsulation option.
Chem. Phys. Lett. 545 (2012) 44-55.
- 19) **F. Y. Naumkin** and D. J. Wales, Beryllium cluster cages endohedrally doped by hydrogen:
 $H_2@Be_n$ ($8 \leq n \leq 14$). (*Featured on inside cover.*)
Int. J. Quantum Chem. 112 (2012) 3068-3075.
- 20) **F. Y. Naumkin** and D. J. Wales, H_2 molecules encapsulated in extended Be_n cluster cages:
Towards light-metal nanofoams for hydrogen storage.
J. Phys. Chem. A 115 (2011) 12105-12110.
- 21) F. Calvo, **F. Y. Naumkin**, and D. J. Wales,
Interplay between charge and vibrational delocalization in cationic helium clusters.
J. Chem. Phys. 135 (2011) 124308.
- 22) **F. Y. Naumkin**, Complexes of Be and Mg with unsaturated hydrocarbon molecules: inter-
and intramolecular cooperativity of binding.
Chem. Phys. Lett. 499 (2010) 203-208.
- 23) G. Kochhar, **F.Y. Naumkin**, Insertion complexes of an organic molecule trapped in ion-pairs.
New J. Chem. 34 (2010) 2932-2936.
- 24) P. McNelles, **F. Y. Naumkin**, A small molecule in metal cluster cages: $H_2@Mg_n$ ($n=8-10$).
Phys. Chem. Chem. Phys. 11 (2009) 2858-2861.
- 25) **F. Y. Naumkin**,
Towards gold shells shaped by carbon cores: From a gold cage to a core-shell aurocarbon.
Chem. Phys. Lett. 466 (2008) 44-49.
- 26) **F. Y. Naumkin**, Trapped-molecule charge-transfer complexes with huge dipoles: $M-C_2F_6-X$
($M = Na$ to Cs , $X = Cl$ to I)
Phys. Chem. Chem. Phys. 10 (2008) 6986-6990.
- 27) **F.Y. Naumkin**,
Flat-structural motives in small alumino-carbon clusters C_nAl_m ($n=2-3$, $m=2-8$).
J. Phys. Chem. A 112 (2008) 4660-4668.

- 28) **F. Y. Naumkin**, Doping-induced structure and property variations in alkali-cluster halides: Li_{13}F & Li_{13}F_2 . (*Invited paper* in a Special issue on Alkali metal clusters)
J. Comput. Meth. Sci. & Eng. 7 (2007) 463-474.
- 29) H. Leung and **F. Y. Naumkin**, Induced super-halogen behaviour of metal moieties in halogen-doped clusters: $\text{Li}_n\text{I}^{(-)}$ and $\text{Al}_n\text{I}^{(-)}$, $n = 13, 1, 2, 3$.
J. Phys. Chem. A 110 (2006) 13514-13520.
- 30) **F. Y. Naumkin**,
Metastable intermolecular charge-transfer complexes with a pentavalent carbon atom.
J. Phys. Chem. A 110 (2006) 11392-11395.
- 31) **F. Y. Naumkin**, Induced hyper-valence of carbon in metal-fluorocarbon complexes.
Phys. Chem. Chem. Phys., 8 (2006) 4402-4404.
- 32) **F. Naumkin**, Nano-jewellery: C_5Au_{12} – a gold-plated diamond at molecular level.
Phys. Chem. Chem. Phys. 8 (2006) 2539-2545.
[*Highlighted in the Roy. Soc. Chem. bulletin: Chem. Sci. 3 (2006) C51.]*
- 33) S. Dobrin, J. B. Giorgi, **F. Y. Naumkin**, and J. C. Polanyi, Photoinduced charge-transfer reaction at surfaces: III. $(\text{HF})_2 \cdot \text{Na}_n / \text{LiF}(001) + h\nu$ (640 nm) \rightarrow $(\text{HFF}^-\text{Na}_n^+ / \text{LiF}(001) + \text{H}(g)$.
J. Chem. Phys. 122 (2005) 014705.
- 34) S. Dobrin, X. Lu, **F. Y. Naumkin**, J. C. Polanyi, and J. Yang, Imprinting Br atoms at Si(111) from a SAM of $\text{CH}_3\text{Br}(\text{ad})$, with pattern retention.
Surf. Sci. 573 (2004) L363-368.
[*Highlighted in Chem. & Eng. News 82 (2004) 8.]*
- 35) **F. Y. Naumkin** and F. R. W. McCourt, *Ab initio*-based PES extrapolated using transferable atom-atom potentials, and predicted MW spectrum of the Ar-O_2 ($X^3\Sigma_g^-$) complex.
Mol. Phys. 102 (2004) 37-45.
- 36) S. Dobrin, H. He, **F. Y. Naumkin**, J.C. Polanyi, S.A. Raspopov,
Photoinduced charge-transfer reaction at surfaces. Part II. $\text{HBr} \cdot \text{Na}_n / \text{LiF}(001) + h\nu$ (610 nm) \rightarrow $\text{Br}^-\text{Na}_n^+ / \text{LiF}(001) + \text{H}(g)$
J. Chem. Phys. 119 (2003) 9795-9803.
- 37) **F. Y. Naumkin**, J. C. Polanyi, D. Rogers, W. Hofer, and A. Fisher,
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Surf. Sci. 547 (2003) 324-334.
- 38) **F. Y. Naumkin**, J. C. Polanyi, and D. Rogers,
Reaction of chlorinated benzenes with $\text{Si}(100)2 \times 1$: a theoretical study.
Surf. Sci. 547 (2003) 335-348.
- 39) **F. Y. Naumkin** and D. J. Wales, Diatomics-in-molecules potentials incorporating *ab initio* data: Application to ionic, Rydberg-excited, and molecule-doped rare gas clusters.
Comp. Phys. Commun. 145 (2002) 141-155.
- 40) J. N. Murrell, **F. Y. Naumkin**, and C. R. Griffiths,
The structures and stabilities of mixed inert gas cluster ions: NeHe_n^+ and ArHe_n^+ .
Mol. Phys. 99 (2001) 115-132.
- 41) **F. Y. Naumkin**,
Binding in the $\text{Ar-I}_2(X^1\Sigma_g^+)$ complex: A challenge for theory and experiment.
ChemPhysChem 2 (2001) 121-125 [@ Angew. Chemie 40 (2001) No. 4].
- 42) **F. Y. Naumkin** and D. J. Wales, Molecule-doped rare gas clusters: Structure and stability of Ar_nNO ($X^2\Pi_{1/2, 3/2}$), $n \leq 25$, from new *ab initio* potential energy surfaces of ArNO .
Mol. Phys. 98 (2000) 219-229.
- 43) **F. Y. Naumkin**,
Transition intensities in rare gas triatomic ions: DIM versus point-charge approximation.
Chem. Phys. 252 (2000) 301-314.

- 44) J. B. Giorgi, **F. Y. Naumkin**, J. C. Polanyi, S. A. Raspopov, N. S.-K. Sze, Surface aligned photochemistry: Photodissociation of Cl₂ and Cl₂···Cl adsorbed on LiF (001) surface. *J. Chem. Phys.* 112 (2000) 9569-9581.
- 45) **F. Y. Naumkin**, DIM models for RgX₂⁻ systems: Suppressed influence of spin-orbit coupling and induced multipole effects for the Ar-I₂⁻ interaction. *Chem. Phys.* 240 (1999) 79-92.
- 46) N. L. Doltsinis, P. J. Knowles, and **F. Y. Naumkin**, Induced dipole - induced dipole interactions in Ar_n⁺ clusters. *Mol. Phys.* 96 (1999) 749-755.
- 47) **F. Y. Naumkin** and F. R. W. McCourt, Is the Ar-Br₂(X ¹Σ_g⁺) Van der Waals complex linear rather than T-shaped? A study in terms of *ab initio*-based potential energy surfaces. *Mol. Phys.* 96 (1999) 1043-1049.
- 48) **F. Y. Naumkin** and D. J. Wales, Rydberg excitations in rare gas atomic clusters: Structure and electronic spectra of Ar_n* (3 ≤ n ≤ 25). *Mol. Phys.* 96 (1999) 1295-1304
- 49) **F. Y. Naumkin**, An “electrons-in-molecule” model for atom-atom representation of atom-molecule potentials, with application to the Ar-B₂(X ³Σ_g⁻) complex. *Phys. Chem. Chem. Phys.* 1 (1999) 3949-3954.
- 50) **F. Y. Naumkin**, Single- versus multi-state DIM model for RgX₂ systems: On the influence of spin-orbit coupling on Ar-I₂ potentials. *Chem. Phys.* 226 (1998) 319-335.
- 51) **F. Y. Naumkin** and D. J. Wales, Structure and properties of Ne_n⁺ clusters. *Mol. Phys.* 93 (1998) 633-648.
- 52) **F. Y. Naumkin** and F. R. W. McCourt, Contributions of the two conformers to the MW spectrum and scattering cross section of the He-Cl₂ van der Waals system, evaluated from an *ab initio* potential energy surface. *J. Chem. Phys.* 108 (1998) 9301-9312.
- 53) **F. Y. Naumkin** and D. J. Wales, Influence of the atom-atom interaction anisotropy on the structure and stability of Ar_nCl₂ clusters. *Chem. Phys. Lett.* 290 (1998) 164-170.
- 54) **F. Y. Naumkin** and F. R. W. McCourt, *Ab initio*-based potential energy surfaces, microwave spectrum, and scattering cross section of the ground state Ne-Cl₂ system. *J. Chem. Phys.* 109 (1998) 1271-1284.
- 55) **F. Y. Naumkin** and F. R. W. McCourt, On the influence of rare gas atom - chlorine ion potentials on the ground state Rg-Cl₂ interaction. *Chem. Phys. Lett.* 292 (1998) 63-70.
- 56) **F. Y. Naumkin** and F. R. W. McCourt, *Ab initio*-based potential energy surfaces and predicted microwave spectra of the Ar-I₂(X ¹Σ_g⁺) Van der Waals complex. *Chem. Phys. Lett.* 294 (1998) 71-78.
- 57) W. Jäger, Y. Xu, G. Armstrong, M. C. L. Gerry, **F. Y. Naumkin**, F. Wang, and F. R. W. McCourt, Microwave spectra of NeN₂ van der Waals complex: Experiment and theory. *J. Chem. Phys.* 109 (1998) 5420-5432.
- 58) **F. Y. Naumkin** and F. R. W. McCourt, A nontypical atom-diatom van der Waals interaction: Ar-C₂. *J. Chem. Phys.* 107 (1997) 1185-1194
- 59) **F. Y. Naumkin**, Molecular versus atom-atom interaction anisotropy in the case of the Ar-N₂ van der Waals system. *Molecular Physics* 90 (1997) 875-888.

- 60) **F. Y. Naumkin** and F. R. W. McCourt,
A study of the ArCl₂ van der Waals complex: *Ab initio*-based potential energy surfaces, the relative stability of conformers, and the “hidden” microwave spectrum.
J. Chem. Phys. 107 (1997) 5702-5713.
- 61) **F. Y. Naumkin**, The ArClF van der Waals complex as an example of how atoms inside a molecule interact with those outside.
Chem. Phys. 213 (1996) 33-44
- 62) **F. Y. Naumkin** and P. J. Knowles, Combined empirical - model - *ab initio* potentials for complexes of rare gas atoms with diatomic molecules.
In: Femtochemistry - Ultrafast Chemical and Physical Processes in Molecular Systems, Ed. M. Chergui, World Scientific, 1996, pp.94-98.
- 63) **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
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- 64) **F. Y. Naumkin**, P. J. Knowles, and J. N. Murrell,
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- 66) Abarenov A. V., **Naumkin F. Y.**, Pevgov V. G.
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- 67) **Naumkin F. Y.**, Pevgov V. G.
Electronic states of triatomic rare gas excimer molecules
Soviet Physics - Lebedev Institute Reports (USA), 9 (1989) 64-67.
- 68) **Naumkin F. Y.**, Pevgov V. G.
Application of the DIM method to calculation of R₃⁺ (R = Ne - Xe) triatomic ion potentials
Soviet Physics - Lebedev Institute Reports (USA), 10 (1989) 4-7.
- 69) **Naumkin F. Y.**
Photoabsorption by triatomic rare gas ions
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- 70) **Naumkin F. Y.**
Matrix elements calculation within the diatomics-in-molecules method
Soviet Physics - Lebedev Institute Reports (USA), 8 (1991) 27-31.
- 71) **Naumkin F. Y.**
Analytic solution for R₂RX* molecule potentials
Soviet Physics - Lebedev Institute Reports (USA), 8 (1991) 42-45.
- 72) **Naumkin F. Y.**
Radiative transition moments of R₃* (R = Ne, Ar, Kr)
Bulletin of Lebedev Physical Institute (USA), 9 (1992) 11-14.
- 73) **Naumkin F. Y.**
Emission of Ne₃*, Ar₃*, Kr₃* molecules
Bulletin of Lebedev Physical Institute (USA), 9 (1992) 19-24.
- 74) Abarenov A. V., **Naumkin F. Y.**, Pevgov V. G.
Modification of the diatomics-in-molecules method for calculation of large molecules consisting of atoms with one external s-electron (brief version)
Bulletin of Lebedev Physical Institute (USA), 9 (1992) 15-18.

- 75) Abarenov A. V., **Naumkin F. Y.**, Pevgov V. G.
Modification of the diatomics-in-molecules method for calculation of large molecules consisting of atoms with one external s-electron (full version)
General Physics Institute Proceedings (Russia), 42 (1993) 131-135.
- 76) **Naumkin F. Y.**, Pevgov V. G.
Energies, transition moments, and photoprocess cross sections of R_3^+ and R_3^* triatomic rare gas molecules
General Physics Institute Proceedings (Russia), 42 (1993) 92-119.
- 77) Abarenov A. V., **Naumkin F. Y.**, Pevgov V. G.
Classical trajectory modelling of vibrational relaxation of $XeCl^*$ molecule on Ar atom
General Physics Institute Proceedings (Russia), 42 (1993) 120-130.

(iii) Articles in refereed conference proceedings

- 1) 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. $LiFCH_3$.
Faraday Discuss. 118 (2001) 191-207
- 2) J. B. Giorgi, T. G. Lee, **F. Y. Naumkin**, J. C. Polanyi, S. A. Raspopov, and J. Wang,
Photoinduced charge-transfer reactions at surfaces: $(HCl)_mNa_n/LiF(001) + h\nu$ (640 nm) \rightarrow
 $(HCl)_{m-1}ClNa_n/LiF(001) + H(g)$.
Faraday Discuss. 117 (2000) 85-97.

Abstracts

- 1) **F. Y. Naumkin** and P. McNelles, Hydrogen molecules in metal cluster cages: Weak bonding and reactions in confined spaces.
Abstracts of Papers of the American Chemical Society 238 (2009) 74-PHYS.
- 2) **F. Y. Naumkin**, G. Kochhar, and P. McNelles, Carbon aurides and hyper-aurides: Usual and unusual hybridization in carbon.
Abstracts of Papers of the American Chemical Society 238 (2009) 38-INOR.
- 3) 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.
Abstracts of Papers of the American Chemical Society 226 (2003) 248-COLL Part 1.
- 4) 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 $LiF(001)$.
Abstracts of Papers of the Am. Chem. Soc. 224 (2002) 280-COLL Part 1.
- 5) S. A. Raspopov, N. S. K. Sze, **F. Y. Naumkin**, J. B. Giorgi, and J. C. Polanyi,
Photoinduced dynamics of Cl_3 radical-molecule complex prepared and studied at $LiF(001)$ surface. Abstracts of Papers of the Am. Chem. Soc. 223 (2002) 093-PHYS Part 2.
- 6) 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, $M\cdots XR + h\nu \rightarrow [M^*\cdots XR] \rightarrow [M^+\cdots XR^-] \rightarrow$ products: Results for $M = Li$, $X = F$, $R = CH_3$ or H .
Abstracts of Papers of the Am. Chem. Soc. 219 (2000) 053-COMP Part 1.
- 7) 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, $M\cdots XR + h\nu \rightarrow [M^*\cdots XR] \rightarrow [M^+\cdots XR^-] \rightarrow$ products ($X = F, Cl, Br$; $R = H$ or CH_3).
Abstracts of Papers of the Am. Chem. Soc. 218 (1999) 388-PHYS Part 2.

CONFERENCES REPORTS

- 1) **F. Y. Naumkin**, S. Kerr, B. Cochrane
Highly polar supramolecular species with enhanced IR activity.
47th IUPAC Congress, Paris, France, Jul 7-12, 2019. (*Talk*)
- 2) **F. Y. Naumkin**, S. Kerr, B. Cochrane
Dipoles inside of dipoles: Highly polar supramolecular species
7th EuCheMS Congress, Liverpool, UK, Aug 26-30, 2018. (*Talk*)
- 3) **F. Y. Naumkin** and B. Cochrane
Uncommon molecular insertion complexes: non-dipoles and dipoles inside of dipoles.
11th WATOC Congress, Munich, Germany, Aug 27 - Sep 1, 2017. (*Talk*)
- 4) **F. Y. Naumkin**, B. Cochrane, S. Kerr
Dipoles inside dipoles: Uncommon insertion complexes of polar molecules.
53rd Symposium on Theoretical Chemistry, Basel, Switzerland, Aug 21-25, 2017.
- 5) **F. Y. Naumkin**, Stability and polarity of the insertion complexes of fluorinated molecules in ion-pairs. 100th Canadian Chemistry Conference, Toronto, Canada, May 28 - Jun 1, 2017. (*Talk*)
- 6) **F. Y. Naumkin** and S. Kerr, Dipoles inside of dipoles: Uncommon insertion complexes of polar molecules.
100th Canadian Chemistry Conference, Toronto, Canada, May 28 - Jun 1, 2017. (*Talk*)
- 7) B. Irving and **F. Y. Naumkin**,
Evolution of properties of metal cluster cages via encapsulation of molecular dopants.
18th ISSPIC Meeting, Jyväskylä, Finland, Aug 14-19, 2016.
- 8) B. Cochrane and **F. Y. Naumkin**, Molecules in Ion-pair Traps: Reshaping and Linking.
99th CSC Meeting, Halifax, Canada, June 5-9, 2016. (*Talk*)
- 9) **F. Y. Naumkin**, K. Fisher, B. Irving, and D. J. Wales,
Charge-controlled structural dynamics of molecular systems.
1st MOLIM General Meeting, Paris, France, Aug 27-29, 2015.
- 10) **F. Y. Naumkin** and K. Fisher,
Metal-organic molecular units with charge-controlled structures.
98th CSC meeting, Ottawa, Canada, June 13-17, 2015. (*Talk*)
- 11) **F. Y. Naumkin** and D. J. Wales, Encapsulation of atomic hydrogen in metal cluster cages and their assemblies: Towards hydrogen-filled nanofoams.
98th CSC meeting, Ottawa, Canada, Jun 13-17, 2015.
- 12) **F. Y. Naumkin**, Core-shell metallocarbons: Property alteration and structure control.
98th CSC meeting, Ottawa, Canada, June 13-17, 2015. (*Talk*)
- 13) **F. Y. Naumkin** and D. J. Wales, Towards light-metal nanofoams for hydrogen storage: Trapping hydrogen in assemblies of metal cluster cages.
98th CSC meeting, Ottawa, Canada, June 13-17, 2015.
- 14) **F. Y. Naumkin**,
Core-shell metallocarbons: Property alteration and charge-controlled structural dynamics.
20th MOLEC European Conference, Gothenburg, Sweden, Aug. 2014.
- 15) **F. Y. Naumkin** and K. Fisher,
Electronic-perturbation induced structural dynamics of metal-organic molecular sandwiches.
20th MOLEC European Conference, Gothenburg, Sweden, Aug. 2014.
- 16) B. J. Irving and **F. Y. Naumkin**, Al-kanes and Al-kenes.
97th Canadian Chemistry Conference, Vancouver, Canada, June 2014. (*Talk*)
- 17) **F. Y. Naumkin**, Molecular vs atomic encapsulation of hydrogen in metal cluster-cage assemblies. VIIIth Congress of the Int. Society of Theor. Chem. Physics, Budapest, Hungary, Aug. 2013. (*Talk*)

- 18) **F. Y. Naumkin**,
Metal-organic molecular interfaces: Options for induced structure manipulation.
44th IUPAC World Chemistry Congress, Istanbul, Turkey, Aug. 2013. (*Talk*)
- 19) **F. Y. Naumkin** and D. J. Wales,
Hydrogen in metal cluster-cage assemblies: molecular vs atomic encapsulation options.
44th IUPAC World Chemistry Congress, Istanbul, Turkey, Aug. 2013. (*Talk*)
- 20) **F. Y. Naumkin**, Metal-organic molecular units for induced structure manipulation.
28th Symposium of Chemical Physics, Waterloo, Nov. 2012. (*Talk*)
- 21) **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*)
- 22) **F. Y. Naumkin** and D. J. Wales,
Hydrogen in light-metal cage assemblies: Towards a nanofoam storage.
4th EuCheMS meeting, Prague, Czech Republic, Aug 2012.
- 23) **F. Y. Naumkin** and G. Kocchar,
Metal-mediated molecular junctions: a computational design.
94th Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
- 24) **F. Y. Naumkin**, Shape design and property alterations of aurocarbon core-shell species.
94th Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
- 25) **F. Y. Naumkin**,
Computational exploration of cluster species with molecular cores inside metal-atom shells.
94th Canadian Chemistry Conference, Montreal, Canada, June 2011. (*Talk*)
- 26) **F. Y. Naumkin** and D. J. Wales,
Hydrogen@metal core-shell cluster species: towards efficient in-cage storage.
94th Canadian Chem. Conf., Montreal, Canada, June 2011. (*Talk*)
- 27) **F. Y. Naumkin** and G. Kocchar,
Organic molecules linked by metal atoms: sandwich- and trap-type interfaces.
94th Canadian Chemistry Conf., Montreal, Canada, June 2011. (*Talk*)
- 28) **F. Y. Naumkin**, Computational design of metal-mediated molecular junctions.
3rd EuCheMS Congress of Chemistry, Nurnberg, Germany, Aug.-Sep. 2010. (*Talk*)
- 29) **F. Y. Naumkin** and G. Kocchar,
Un/usual coordination of carbon in hyper/metallide CM_n species.
25th Symposium of Chemical Physics, Waterloo, Nov. 2009. (*Talk*)
- 30) **F. Y. Naumkin** and P. McNelles,
Hydrogen in metal cluster cages: weak bonding and reactions in confined spaces.
238th ACS National Meeting, Washington, U.S., August 2009. (*Talk*)
- 31) G. Kochhar, P. McNelles, **F. Y. Naumkin**,
Carbon aurides and hyper-aurides: usual and unusual coordination of carbon.
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- 32) **F. Y. Naumkin** and P. McNelles,
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- 33) G. Kochhar, P. McNelles, **F. Y. Naumkin**,
Carbon aurides and hyper-aurides: unusual coordination of carbon and other properties.
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- 34) **F. Y. Naumkin** and P. McNelles,
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- 35) G. Kochhar, P. McNelles, **F. Y. Naumkin**,
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- 36) **F. Y. Naumkin** and P. McNelles,
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- 37) **F. Y. Naumkin**, Gold shells shaped by carbon cores: From Au₁₈ cage to C₁₀Au₁₈ aurocarbon.
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- 38) **F. Y. Naumkin**, Unusual structural and electronic features of small C_nAl_m clusters.
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- 39) **F. Y. Naumkin**, Dividing the charge and conquering the valence: Novel trapped-molecule complexes with penta-valent carbon.
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- 40) **F. Y. Naumkin**,
Metal cluster-cages shaped by molecular fillers: Towards flexible design of parameters.
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- 41) **F. Y. Naumkin**, High-energy intermolecular sandwiches: harpooning through a molecule.
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- 42) **F. Y. Naumkin**,
Criminal applications of Quantum Mechanics: Putting molecules behind nano-bars.
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- 43) **F. Y. Naumkin**, Nano-jewellery: C₅Au₁₂ – a gold-plated diamond at molecular level.
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- 44) **F. Y. Naumkin** and H. Leung,
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