Yifat Miller - Curriculum Vitae

Education:

1997	-	B.Sc. (Chemistry), Hebrew University, Jerusalem
2002	-	M.Sc. (Computational Physical Chemistry), Hebrew University, Jerusalem
2007	-	Ph.D. (Computational Physical Chemistry), Hebrew University, Jerusalem (Thesis: Vibrational spectroscopy and reaction dynamics of atmospheric molecules)

Research publications:

1. **Miller, Y.**, Ma, B., and Nussinov, R.: Metal binding sites in amyloid oligomers: complexes and mechanisms. Coord. Chem. Rev., in press, 2012.

2. Liessmann M., **Miller Y.**, Gerber R.B., and Abel B.: Reaction of OH and NO at low temperatures in the presence of water: The role of clusters. Z. Phys. Chem. 225: 1129-1144, 2011.

3. **Miller Y**, Ma B, and Nussinov R.: Synergistic interactions between repeats in tau protein and Aβ amyloids may be responsible for accelerated aggregation via polymorphic states. Biochemistry, 50(23):5172-81, 2011.

4. **Miller, Y.**, Ma, B., and Nussinov R.: Stability of fibrils and annular species using all-atom molecular dynamics (MD) simulations in solvent: insight into polymorphism. Derreumaux, P. (Ed.): Alzheimer's disease: Molecular Basis of Amyloid-beta protein aggregation and fibril formation Insights into low molecular weight and cytotoxic aggregates from computer simulations. Imperial College press, 2011, Chapter 3.

5. Parthasarathy, S., Long, F., **Miller, Y.**, Xiao, Y., McElheny, D., Thurber, K., Ma, B., Nussinov, R., and Ishii, Y.: Molecular-level examination of Cu^{2+} binding structure for amyloid fibrils of 40-residue Alzheimer's β by solid-state NMR spectroscopy. J. Am. Chem. Soc. 133: 3390-3400, 2011.

6. **Miller, Y.**, Ma, B., and Nussinov, R.: The unique Alzheimer's β-amyloid triangular fibril has a cavity along the fibril axis under physiological conditions. J. Am. Chem. Soc. 133, 2742-2748, 2011.

7. Shmilovits-Ofir, M., **Miller, Y.**, and Gerber R.B.: Conformational transitions of glycine induced by vibrational excitation of the O-H stretch. Phys. Chem. Chem. Physics, 2010, DOI: 10.1039/C0CP01385D. ***Advance article in a special issue***

8. **Miller, Y.**, Ma, B., Tsai, C.-J., and Nussinov, R.: The hollow core of Alzheimer $A\beta_{42}$ amyloid observed by cryoEM is relevant at physiological pH. Proc. Natl. Acad. Sci. USA, 107:14128-14133, 2010.

9. **Miller, Y.**, Ma, B., and Nussinov, R.: Zinc ions promote Alzheimer Aβ aggregation via population shift of polymorphic states. Proc. Natl. Acad. Sci. USA, 107: 9490-9495, 2010.

10. **Miller, Y.**, Ma, B., and Nussinov, R: Polymorphism in Alzheimer Aβ amyloid organization reflects conformational selection in a rugged energy landscape. Chem. Rev., **DOI:** 10.1021/cr900377t, 2010.

11. **Miller, Y.**, Ma, B., and Nussinov, R.: Polymorphism of Alzheimer's $A\beta_{17-42}$ (p3) oligomers: The importance of the turn location and its conformation. Biophys. J. 97(4): 1168-1177, 2009.

12. **Miller, Y.**, Thomas, J.L., Kemp, D.D., Finlayson-Pitts, B.J., Gordon, M.S., Tobias, D.J. and Gerber, R.B.: Structure of large nitrate-water clusters at ambient temperatures: Simulations with effective fragment potentials and force fields with implications for atmospheric chemistry. J. Phys. Chem. A, 113 (46): 12805, 2009.

13. **Miller, Y.**, Finlayson-Pitts, B. J., and Gerber, R. B.: Ionization of N_2O_4 in contact with water: Mechanism, timescales and atmospheric implications. J. Am. Chem. Soc. 131: 12180, 2009. ***Cover article.***

14. Link, O., Vöhringer-Martinez, E., Lugovoj, E., Liu, Y., Siefermann, K., Faubel, M., Grubmuller, H., Gerber, R.B., **Miller, Y.**, Abel, B.; Ultrafast phase transitions in metastable water near liquid interfaces. Faraday Discuss. 141: 67-79, 2009. DOI: 10.1039/b811659h

15. Kamboures, M. A., Raff, J. D., **Miller, Y.**, Philips, L. F., Finlayson-Pitts, B. J., and Gerber, R. B.: Complexes of HNO_3 and NO_2 and N_2O_4 and their potential role in atmospheric HONO formation. Phys. Chem. Chem. Phys. 10: 6019, 2008.

16. Wolf, I., Shapira, A., Giniger, R., **Miller, Y.**, Gerber, R. B., and Cheshnovsky, O.: Critical size for intracluster proton transfer from water to an anion. Communication. Angew. Chem. Int. Ed. 47: 10.1002/ange.200800542, 2008.

17. **Miller, Y.** and Gerber, R. B.: Dynamics of proton recombination with NO_3^- anions in water clusters. Phys. Chem. Chem. Phys. 10: 1091, 2008. ***Cover communication article.***

18. **Miller, Y.**, Vaida, V., and Gerber, R. B.: Photodissociation yields for high vibrational excitations of H_2SO_4 in atmospheric conditions. Geophys. Res. Lett. 34: Art No. L16820, 2007. ***Featured as a scientific highlight article.***

19. **Miller, Y.**, Chaban, G. M., Zhou, J., Asmis, K. R., Neumark, D. M., and Gerber, R. B.: Vibrational spectroscopy of $SO_4^{2-} \bullet (H_2O)_n$ cluster, n=1.5: Harmonic and anharmonic calculations, and experiment. J. Chem. Phys. 127: Art No. 094305, 2007.

20. Ramazan, K. A., Wingen, L. M., **Miller, Y.**, Chaban, G. M., Gerber, R. B., Xantheas, S., and Finlayson-Pitts, B. J.: A new experimental and theoretical approach to the heterogeneous hydrolysis of NO_2: The key role of molecular nitric acid and its complexes with water. J. Phys. Chem. A 110: 6886, 2006.

21. **Miller, Y.** and Gerber, R. B.: Dynamics of vibrational overtone excitations of H_2SO_4, H_2SO_4-H_2O: Hydrogen – Hopping and photodissociation processes. J. Am. Chem. Soc. 128: 9594, 2006.

22. **Miller, Y.**, Chaban, G. M., Finlayson-Pitts, B. J., and Gerber, R. B.: Photochemical processes-induced by vibrational overtone excitations: Dynamics simulations for cis HONO, trans HONO, HNO_3 and HNO_3-H_2O. J. Phys. Chem. A 110: 5342, 2006.

23. Gerber, R. B., Chaban, G. M., Brauer, B., and **Miller, Y.**: First principles calculations of anharmonic vibrational spectroscopy of large molecules. In Dykstra, C. E., Kim, K. S., Fleming, G., and Scuseria, G. E. (Eds.): Theory and Applications of Computational Chemistry: The First 40 Years. Amsterdam, Netherlands, Elsevier Publications, 2005, Chapter 9, pp. 165-193

24. **Miller, Y.**, Chaban, G. M., and Gerber, R. B.: Ab initio vibrational calculations for H_2SO_4 and H_2SO_4-H_2O: Spectroscopy and the nature of the anharmonic couplings. J. Phys. Chem. A 109: 6565, 2005.

25. **Miller, Y.**, Chaban, G. M., and Gerber, R. B.: Theoretical study of anharmonic vibrational spectra of HNO_3, HNO_3-H_2O, HNO_4, cis HONO and trans HONO: Fundamental, overtone and combination excitations. Chem. Phys. 313: 213, 2005.

26. **Miller, Y.**, Fredj, E., Harvey, J. N., and Gerber, R. B.: UV spectroscopy of large water clusters: Model and Calculations for $(H_2O)_n$, n=8, 11, 20, 40 and 50. J. Phys. Chem. A 108: 4405, 2004.

Participation in research projects:

2008-2011 - Postdoctoral Fellow, Center for Cancer Research (CCR) Nanobiology Program, National Cancer Institute (NCI), National Institutes of Health (NIH), Frederick, MD, USA. **Research projects:** Polymorphism of Aβ amyloids and the effect on metal ions on Aβ aggregation.

2010-2011: **Collaborator:** Prof. Yoshitaka Ishii (University of Illinois, Chicago, USA) **Research project:** "Polymorphism of Aβ-Cu^{2+} complexes".

2010-2011: **Collaborator:** Prof. Joel P. Schneider (NCI-Frederick, NIH, USA) **Research project:** "Modeling of the self-assembly of the β-hairpin peptide MAX1".

2002-2007: Ph.D., Hebrew University, Jerusalem. **Thesis:** "Vibrational spectroscopy and reaction dynamics of atmospheric molecules"

2007-2008: **Collaborator:** Prof. Bernd Abel (University of Göttingen**,** Germany) **Research project:** Ultrafast phase transitions in metastable water near liquid interfaces.

2007-2008: **Collaborators:** Prof. Douglas J. Tobias (University of California Irvine, CA, USA) and Prof. Mark S. Gordon (Iowa state university, IW, USA). **Research project:** Simulations of nitrate ions in water.

2007: **Collaborator:** Prof. Ori Cheshnovsky (Tel-Aviv University, Israel). **Research project:** Proton transfer in water clusters.

2006: **Collaborator:** Prof. Daniel M. Neumark (UCSF, CA, USA). **Research project:** IR spectroscopy of sulfate ions in water.

2006: **Collaborator:** Prof. Veronica Vaida (University of Boulder, CO, USA). **Research project:** Photodissociation of sulfuric acid under atmospheric conditions.

2005 : Research Visitor, AirUCI, Department of Chemistry, University of California Irvine, CA, USA. **Collaborator:** Prof. Barbara J. Finlayson-Pitts. **Research projects:** IR spectroscopy of atmospheric molecules and the role of nitric acid in water.

2005: **Collaborators:** Prof. Barbara J. Finlayson-Pitts (UCI, CA, USA), Dr. Galina Chaban (NASA Ames lab, CA, USA), Prof. Sotiris Xantheas (Pacific Northwest National Laboratory, WA). **Research project:** IR spectroscopy of nitrate and nitric acid in water interface.

1998-2002: M.Sc., Hebrew University, Jerusalem. **Thesis:** "UV spectroscopy of large water clusters: Model and simulations".

Awards, honors, fellowships and other scientific recognitions:

2011: Platinum highlight article: **Miller, Y.**, Ma, B., and Nussinov, R.: The unique Alzheimer's β-amyloid triangular fibril has a cavity along the fibril axis under physiological conditions. J. Am. Chem. Soc. 133, 2742-2748, 2011. ***Selected by the Office of Scientific Operations of "The Poster newsletter", NCI-Frederick, NIH.***

2008-2011: Intramural Research Program fellowship of the NIH, National Cancer Institute, Center for Cancer Research

2008-2011: HFSP Fellowship Award (2008-2011) – Declined

2002-2006: Graduate Research Klein Fellowship, Chemistry Department, Hebrew University, Jerusalem

1991-1992: Scholarship for Excellence for Graduate Studies, Hadassah College, Jerusalem

Research grants:

2012-2015: Marie Curie Reintegration Grant, "Insight into the synergistic interactions between Aβ amyloid, α-synuclein and Tau"

2012-2014: NIH R01 Grant, "The physiological role of carbonic acid and lactic acid as protonating agents of amine and nitrogen bases in model biological environments"

Invited Talks:

1. Miller Y.: Synergistic interaction between amyloidogenic peptides and their effect in amyloid aggregation, Department of Microbiology and Molecular Genetics Hebrew University of Jerusalem, Hadassah Medical School, Jerusalem, March 26, 2011.

2. Miller, Y.: Synergistic interaction between amyloidogenic peptides and their effect in amyloid aggregation, Whilhelm-Ostwald Institute for Physical and Theoretical Chemistry, Universität Leipzig, Leipzig, Germany, Dec 15, 2011.

3. Miller, Y.: Synergistic interaction between amyloidogenic peptides and their effect in amyloid aggregation, Center For Integrated Protein Science Munich, Technische Universität München, Freising, Germany, Dec 13, 2011.

4. Miller, Y.: Synergistic interaction between repeats in tau protein and Aβ amyloids are responsible for accelerated aggregation in Alzheimer's disease, Center for Cancer Research Nanobiology Program, NCI-Frederick, NIH, MD, USA, June 22, 2011.

5. Miller, Y., Ma, B. and Nussinov, R.: Alzheimer's Aβ amyloid tubular fibrils: insight into polymorphism. Biophysical Society 55th Annual Meeting, Baltimore, MD, March 5-9, 2011.

6. Miller, Y.: Tubular protofibrils of Alzheimer's Aβ amyloids are relevant at physiological pH: insight into polymorphism. Center for Cancer Research Nanobiology Program, NCI-Frederick, NIH, October 20, 2010.

7. Miller, Y., Ma, B. and Nussinov, R.: Polymorphism in Alzheimer $A\beta_{17-42}$ (p3): Insight into amyloid arrangements. The 238th ACS National Meeting, Washington, DC , August 16-21, 2009.

8. Miller, Y.: How does zinc promote aggregation in Alzheimer Aβ? Center for Cancer Research Nanobiology Program, NCI-Frederick, NIH, September 16, 2009.

9. Miller, Y.: Polymorphism of Alzheimer Aβ oligomers. Center for Cancer Research Nanobiology Program, NCI-Frederick, October 15, 2008.

10. Raff, J. D., Kamboures, M. K., Miller, Y., Gerber, R. B., and Finlayson-Pitts, B. J.: Complexes of HNO_3 and NO_3^- with NO_2 and its dimmer, and their role in atmospheric HONO formation. 25th Informal Symposium on Kinetics and Photochemical Processes in the Atmosphere, UCLA, CA, February 20, 2008.

11. Gerber, R. B. and Miller, Y.: Ions and charge transfer reactions in water clusters. Diffusion, Solvation and Transport of Protons in Complex and Biological Systems, Eilat, Israel, January 1-17, 2008.

12. Gerber, R. B. and Miller, Y.: Ions and charge transfer reactions in water clusters. AirUCI Workshop, Newport Beach, CA, January 23-24, 2008.

13. Kamboures, M. K., Raff, J. D., Finlayson-Pitts, B. J., Miller, Y., and Gerber, R. B.: Complexes of NO_x: Structure, stability, and possible role in atmospheric chemistry. AirUCI Workshop, Newport Beach, CA, January 23-24, 2008.

14. Gerber, R. B., Miller, Y., and Kamboures, M. A.: Ions and charge transfer reactions in water clusters. ACS National Meeting, Boston, MA, August 19-23, 2007.

15. Gerber, R. B. and Miller, Y.: Ions and charge transfer reactions in water clusters. Conduction in Molecular Systems, Yad Hashmonah, Israel, June 10-11, 2007.

16. Cheshnovsky, O., Wolf, I., Shapira, A., Giniger, R., Miller, Y., and Gerber, R. B.: Size-critical proton-transfer in aqueous clusters of deprotonated aniline. XXII International Symposium on Molecular Beams, Freiburg, Germany, May 27 – June 1, 2007.

17. Charge transfer processes of atmospheric molecules in water clusters. Chemistry Department, Ben-Gurion University, Beer-Sheva, Israel, May 2, 2007.

18. Gerber, B., Miller, Y., and Kamboures, M.: Atmospheric reactions of molecules in water clusters. AirUCI Workshop on Processes at Interfaces, Cristchurch, NZ, December 11-12, 2006.

19. Dynamics of atmospheric reactions at large water clusters: Hydrolysis of N_2O_4 and ionization of HNO_3. AirUCI Workshop on Processes at Interfaces, Laguna Beach, CA, January 26-27, 2006.

20. Gerber, B. and Miller, Y.: Charge transfer processes of molecules in water clusters. Telluride, CA, April 2006.

21. Gerber, B. and Miller, Y.: Dynamics of chemical processes in overtone-excited HNO_3, HNO_3-H_2O, H_2SO_4-H_20. ACS National Meeting, Atlanta, GA, March 2006.

22. Miller, Y. and Gerber, R. B.: Photoinduced proton transfer in HNO_x and H_2SO_4 and the effects of complexation with water. Symposium on Proton Transfer/Transport in H-bonded Solids, Liquids, Clusters and Interfaces, PacificChem 2005, Hawaii, December 15-20, 2005.

23. Vibrational photochemistry: A major mechanism of atmospheric reactions. Environmental Sciences and Energy Research, Weizmann Institute, Rehovot, Israel, November 2005.

24. Vibrational spectroscopy and photoinduced reaction dynamics of atmospheric molecules. AirUCI Meeting, UC Irvine, CA, July 2005.

25. Vibrationally-induced photochemistry of atmospheric molecules. AirUCI Workshop on "Ions and Molecules at Aqueous Interfaces, Prague, Czech Republic, June 25-30, 2005.

26. Vibrational spectroscopy and photoinduced reaction dynamics of atmospheric molecules. Fritz Haber Research Center, Hebrew University of Jerusalem, Israel, May 26, 2005.

27. Gerber, R. B., Miller, Y., and Brown, E.: Overtone spectroscopy and overtone-induced processes in HONO, HNO_3, HNO_4 and HNO_3H_2O. ACS National Meeting, Anaheim, CA, April 2004.

Presentations:

1. Miller, Y., Fredj, E., Harvey, J. N., and Gerber, R. B.: UV spectra of water clusters $(H_2O)_n$, N = 8, 20, 40, 50. Israel TheoChem, Jerusalem, Israel, October 9-10, 2002.

2. Miller, Y., Chaban, G. M., and Gerber, R. B.: Reaction dynamics of atmospherically relevant molecules. 70th Meeting of the Israel Chemistry Society, Tel-Aviv, Israel, February 15-16, 2005.

3. Miller, Y., Chaban, G. M., and Gerber, R. B.: Reaction dynamics of atmospherically relevant molecules. The Fritz Haber Symposium on Biophysical Dynamics, Israel, March 13-14, 2005.

4. Miller, Y., Chaban, G. M., and Gerber, R. B.: Reaction dynamics of atmospherically relevant molecules. 3rd Annual Meeting of Lise Meitner Center, Jerusalem, Israel, June 2, 2005.

5. Wingen, L. M., Ramazan, K. A., Miller, Y., Chaban, G. M., Gerber, R. B., Xantheas, S. S., and Finlayson-Pitts, B. J.: Investigating the heterogeneous chemistry and photochemistry of surface-adsorbed species formed during heterogeneous NO_2 hydrolysis. 23rd Informal Symposium on Kinetics and Photochemical Processes in the Atmosphere, California Institute of Technology, Pasadena, CA, February 15, 2006.

6. Wolf, I., Shapira, A., Giniger, R., Cheshnovsky, O., Miller, Y., and Gerber, R. B.: Critical size effect in solvated ion clusters. James Franck Minerva Program in Laser-Matter Interaction, Tel Aviv, Israel, February 13-15, 2007.

7. Kamboures, M. A., Miller, Y., Chaban, G. M., Finlayson-Pitts, B. J., and Gerber, R. B.: A computational investigation of the chemistry of NO_2 on HNO_3/NO_3 surfaces. iDFT 07 – First Annual DFT Meeting at Irvine/Mini-School and Workshop, Laguna Beach, CA, March 31 – April 1, 2007.

8. Wolf, I., Shapira, A., Giniger, R., Cheshnovsky, O., Miller, Y., and Gerber, R. B.: Critical size effect in solvated ion clusters. XXII International Symposium on Molecular Beams, Frieburg, Germany, May 27 – June 1, 2007.

9. Miller, Y., Ma, B., and Nussinov, R.: Polymorphism in Alzheimer Aβ17-42 (p3): Insight into amyloid arrangements. 4th Annual Cancer Nanobiology Think Tank, NCI-Frederick, May 12, 2009.

10. Miller, Y., Ma, B., Tsai C-J. and Nussinov, R.: Polymorphism in Alzheimer Aβ amyloid organization: Insight into Aβ aggregation. Biophysical Society 54th Annual Meeting, San Francisco, CA, February 20-24, 2010.

11. Miller, Y., Ma, B., Tsai C-J. and Nussinov, R.: Polymorphism in Alzheimer A amyloid organization: Insight into Aβ aggregation. 5th Annual Cancer Nanobiology Think Tank, NCI-Frederick, June 3, 2010.

Invited abstracts:

1. Gerber, R. B., Miller, Y., and Brown, E.: Overtone spectroscopy and overtone-induced processes in HONO, HNO_3, HNO_4, and HNO_3-H_2O. National ACS Meeting, Anaheim, CA, April 2004.

2. Gerber, R. B. and Miller, Y.: Intramolecular and intermolecular proton transfer HNO_3, H_2SO_4, HNO_3 @ $(H_2O)_n$ and H_2SO_4 @ $(H_2O)_n$. PacificChem, Hawaii, December 2005.

3. Gerber, R. B. and Miller, Y.: Dynamics of chemical processes in overtone – Excited HNO_3, HNO_3-H_2O, H_2SO_4, H_2SO_4-H_2O. National ACS Meeting, Atlanta, GA, March 26, 2006.

4. D'Auria, R., Tobias, D.J., Gerber, R.B., Miller, Y. and Xantheas, S.S.: COLL 187-On the interfacial reaction mechanism between OH and Cl-: A detailed description of the mechanism leading to release of gaseous Cl2 from marine aerosols. National ACS Meeting, San Francisco, CA, September 2006.

5. Gerber, R. B., Miller, Y., and Kamboures, M. A.: Atmospheric reactions in water clusters: Mechanisms, dynamics and rates. National ACS Meeting, Boston, MA, August 19-23, 2007.

6. Gerber, R. B. and Miller, Y.: Charge transfer and photochemical reactions in water clusters. National ACS Meeting, Philadelphia, PA, August 2008.

7. Miller, Y., Ma, B. and Nussinov, R.: Polymorphism in Alzheimer $A\beta_{17-42}$ (p3): Insight into amyloid arrangements. The 238th ACS National Meeting, Washington, DC, August 16-21, 2009.

Other professional activities:

2012: Editor in a special issue of E-Journal of Chemistry.

2011: Reviewer for PLoS Computational Biology.

2008-2011: Reviewer for the Journal of the American Chemical Society and other journals of the ACS publications.

2009-2011: Reviewer for the Biophysical Journal.

2003-2006: Teaching Assistant, Pre-academic Studies in Chemistry, Hebrew University, Jerusalem.

1999-2000: Teaching Assistant, Chemistry Department, Open University, Ramat Aviv, Israel.

1997-1999: Teaching Assistant, Chemistry Department, Hebrew University, Jerusalem.

1991-1992: Laboratory Research Assistant, Department of Parasitology, Hebrew University, Hadassah Medical School, Jerusalem.