Dr. Nadia Elghobashi-Meinhardt

Professional background

Feb. 2011 – ongoing	3-year research grant from the Volkswagen Stiftung: "Tackling the reconciliation problem: A quantum mechanical/molecular mechanics (QM/MM) "learn-on-the-fly" study of the effect of aqueous solvent on peptide conformations"
Sep. 2009 – Jan. 2011	*Maternity leave*
Apr. 2007 – Aug. 2009	Researcher Computational Molecular Biophysics at the Interdisciplinary Center for Scientific Computing, University of Heidelberg
Dec. 2005 – Dec. 2006	Post-doctoral fellowship Biophysics group in the Theory Department of the Fritz-Haber-Institute of the Max-Planck-Society, Berlin

Educational background

Jan. 2002 – Oct. 2005	Doctor of Philosophy (Ph.D.) Freie Universität Berlin; Institut für Chemie, Physikalische und Theoretische Chemie Advisor: Prof. Jörn Manz Thesis title: "*Theory of using few-cycle IR and UV laser pulses to control the orientation and selective dissociation of hydrogen-bonded anions*" Grade: *magna cum laude*
Oct. 2000 – Jan. 2002	Master of Science (M.Sc.) Freie Universität Berlin; Institut für Chemie, Physikalische und Theoretische Chemie. Thesis title: "*Quantum Dynamic Calculations of Bond Selective Vibrational Excitation of HOD via Ultrashort IR Laser Pulses*"
Sept. 1995 – Jun. 1999	Bachelor of Science (B.Sc.), Chemistry Stanford University Stanford, California Grade average: 88%
Sept. 1991 – Sept. 1995	University High School Irvine, California Grade average: 100%

Scholarships

Jan. 2005 – June 2005
Berliner Programm zur Förderung der Chancengleichheit für Frauen in Forschung und Lehre
Doctoral research grant

Jan. 2002 – Dec. 2004
Deutsche Forschungsgemeinschaft (DFG)
Doctoral fellowship
Graduate school program: "*Hydrogen Bonding and Hydrogen Transfer* "
Freie Universität Berlin;
Institut für Chemie, Physikalische und Theoretische Chemie
Research area: quantum simulations of laser-driven dynamics of hydrogen bonds in hydrogen-bihalide ions

Oct. 1999 – July 2000
Deutscher Akademischer Austauschdienst (DAAD)
Research grant
Freie Universität Berlin;
Institut für Chemie, Physikalische und Theoretische Chemie
Research area: solid-state NMR (Prof. Limbach)

Employment

Oct. 2000 – Dec. 2001
Computer-aided visualization of results of quantum chemical calculations
Freie Universität Berlin;
Institut für Chemie, Physikalische und Theoretische Chemie.
Software: *Advanced Visual Systems (AVS), Adobe Premiere*

June 1999 – Sept. 1999
Internship at Genencor, Int.
Palo Alto, California
Research area: enzymology

Sept. 1998 – June 1999
Internship at Stanford University;
Dept. of Chemistry, Prof. Trost.
Stanford, California
Research area: organic synthesis

June 1998 – Sept. 1998
Internship at Universitätsklinik, Würzburg
(Stanford-Krupp Internship Program)
Würzburg, Germany
Fields: surgery, dermatology, obstetrics and gynaecology

July 1997 – Sept. 1997
Internship with American Heart Association;
University of California, Irvine;
Dept. of Anatomy and Neurobiology; Prof. Smith
Irvine, California
Research area: olfactory proteins

July 1996 – Sept. 1996
Internship at the University of California, Irvine;
Dept. of Biochemistry and Molecular Biology, Prof. Poulos
Irvine, California
Research area: protein crystallography

PUBLICATIONS

▪N. Elghobashi-Meinhardt, J. C. Smith, A.-N. Bondar, P. Phatak and M. Elstner:
"Hydrogen-bonded network catalysis of ground state *cis*→*trans* isomerization of bacteriorhodopsin's retinal chromophore."
In preparation.

▪N. Elghobashi-Meinhardt, L. González, I. Barth and T. Seideman:
"Few-cycle laser pulses to obtain spatial separation of OHF^- dissociation products."
J. Chem. Phys. **130**, 024310(1)-024310(9) (2009).
Selected for: *Virtual Journal of Ultrafast Science* (Atomic and Molecular Physics), **8**(2), Feb. 2009.

▪N. Elghobashi and L. González:
"A theoretical anharmonic study of the infrared absorption spectra of FHF^-, FDF^-, OHF^-, and ODF^- anions."
J. Chem. Phys. **124**, 174308(1)-174308(12) (2006).

▪N. Elghobashi and L. González:
"Breaking the strong and weak bonds of OHF^- using few-cycle IR+UV laser pulses."
Phys. Chem. Chem. Phys. (Communications), **6**, 4071-4073 (2004). ***Hot article***

▪N. Elghobashi, L. González and J. Manz:
"Quantum model simulations of symmetry breaking and control of bond selective dissociation of FHF^- using IR + UV laser pulses."
J. Chem. Phys. **120**, 8002-8014 (2004).

▪N. Elghobashi, L. González and J. Manz:
"Quantum model simulations for isotope effects of IR + UV laser pulses on symmetry and selective hydrogen bond breaking."
Z. Phys. Chem. **217**, 1577-1596 (2003).

▪N. Elghobashi and J. Manz:
"Separating the photofragments of randomly oriented symmetric reactants by IR+UV laser pulses: quantum simulations for $FHF^- \rightarrow F + FH + e$."
Israel J. Chem., **43**, 293-303 (2003).

▪N. Elghobashi, P. Krause, J. Manz and M. Oppel:
"IR + UV laser pulse control of momenta directed to specific products: Quantum simulations for HOD* → H+OD versus HO+D."
Phys. Chem. Chem. Phys. **5**, 4806-4813 (2003).

▪J.M. Gottfried, N. Elghobashi, S.L.M. Schroeder and K. Christmann:
"Oxidation of gold by oxygen-ion sputtering."
Surf. Sci. **523**, 89-102 (2003).