



Dr. Nadia Elghobashi-Meinhardt

Professional background

- Oct. 2009 – Dec. 2017 Junior Group Leader
Computational Molecular Biophysics / Molecular Modelling
Freie Universität Berlin,
Institut für Chemie, Physikalische und Theoretische Chemie
- Apr. 2007 – Sep. 2009 Researcher
Computational Molecular Biophysics
University of Heidelberg,
Interdisciplinary Center for Scientific Computing
- Dec. 2005 – Dec. 2006 Post-doctoral fellowship
Computational Biophysics
Theory Department,
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.
Thesis title: "*Theory of using few-cycle IR and UV laser pulses to control the orientation and selective dissociation of hydrogen-bonded anions*"
- 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
- Sept. 1991 – Sept. 1995 University High School
Irvine, California

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

Work experience

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

PUBLICATIONS

- F. Krull, G. Korff, N. Elghobashi–Meinhardt and E.–W. Knapp.
“ProPairs: A Data Set for Protein–Protein Docking.” *J. Chem. Inf. Model* **55**(7), 1495–1507 (2015).

- N. Elghobashi–Meinhardt.
“Niemann–Pick Type C Disease: A QM/MM study of conformational changes in cholesterol in the NPC1(NTD) and NPC2 binding pockets.” *Biochem.* **53**(41), 6603–6614 (2014).

- Xiaohu Hu, N. Elghobashi–Meinhardt, D. Gembris and J. C. Smith.
“Response of Water to Electric Fields at Temperatures below the Glass Transition: A Molecular Dynamics Analysis.” *J. Chem. Phys.* **135**, 134507(1)– 134507(10) (2011).

- 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 the Virtual Journal of Ultrafast Science, Vol. 8(2)**)

- 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⁻ → 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).