Ab initio modeling of primary processes in photosynthesis : protein induced activation of bacteriochlorophylls for efficient light harvesting and charge separation

Wawrzyniak, P.K.

Curriculum Vitae

In October 1999, after *cum laude* graduation from I Liceum Ogólnokształcące in Jastrzębie Zdrój I started chemistry studies at the University of Wrocław. Right from the beginning I chose to follow additional teacher training offered as optional integration into the chemistry programme. Starting from second year of studies, I was a researcher trainee under guidance of Dr. Sławomir Berski in the Theoretical Modeling of Chemical Processes Group led by Prof. Dr. Zdzisław Latajka. Also from the second year until graduation, I was receiving University of Wrocław Scientific Scholarship granted for study results. In winter 2002/2003 I spent five months in the Solid State Spectroscopy and Photochemistry group of Prof. Markku Räsänen as Socrates/Erasmus student, doing a research project under supervision of Doc. Dr. Jan Lundell on interactions between formic acid and argon. After coming back to Poland, I continued this work in the group of Prof. Latajka with Dr. Jarosław J. Panek and Doc. Dr. Jan Lundell as supervisors. The project evolved into three publications in scientific journals and Master Thesis *"Formic Acid Complex with Noble Gases: an Ab Initio Quantum Theory Approach"*. In June 2004, I defended the thesis and graduated from the University of Wrocław with M.Sc. degree in chemistry.

In October 2004 I started my Ph.D. project in the Solid-State NMR group at the Leiden University, under guidance of Dr. Francesco Buda and Prof. Dr. Huub J.M. de Groot. During this time I participated in a number of scientific and management courses. These include *"Photophysics, Photochemistry and Photobiology"* (2007) in Amsterdam; *"Winter School on Theoretical Chemistry and Spectroscopy"* (2004, 2005) in Han-sur-Lesse; *"Molecular*

Modeling and the workshop on Computational Photochemistry and Photobiology" (2005) in Amsterdam and *"Self-Organization and the Transition to Life"* (2004) in Leiden. I had lots of opportunities to be on the other side of a classroom as well, assisting in practica of *Molecular Modeling* (2005–2008) and various sorts of *Quantum Chemistry* (2005–2006) and *Computational Chemistry* (2006) courses. I had an opportunity to present my work on many international conferences and meetings through posters and oral communications. Notably, I was one of the speakers at *"Progress in ab initio modeling of biomolecules: methods and applications"* workshop held in 2006 in Leiden and *"Winter School on Theoretical Chemistry and Spectroscopy 2005"* in Han-sur-Lesse. The poster presentations include among others the meetings: *"CBB Workshop Clean Solar Fuels"* (2008) in Amsterdam; *"Solar Energy and Artificial Photosynthesis"* (2007) in London and *"Multi-scale modeling: Electrons, Molecules and (Bio)Materials"* (2006) in Amsterdam. I had also pleasure to be the chairman of SSNMR group seminar series (2007–2008) and Ph.D. representative for the group staff board (2008–2009).

List of Publications

"Origin of Asymmetry in the Special Pair of Bacterial Reaction Center"
P.K. Wawrzyniak, M. Beerepoot, H.J.M. de Groot, F. Buda
manuscript submitted to Phys. Chem. Chem. Phys.

"Hydrogen-bonded water enhances the electron charge donation in bacteriochlorophyll-histidine complexes of bacterial reaction centers"
P.K. Wawrzyniak, H.J.M. de Groot, F. Buda
manuscript submitted to Photosynth. Res.

"NMR secondary shifts of a light-harvesting 2 complex reveal local backbone perturbations induced by its higher-order interactions"
A. Pandit, P.K. Wawrzyniak, A.J. van Gammeren, F. Buda, S. Ganapathy, H.J.M. de Groot
Biochem., 2010, 49, 478–486

"Differential charge polarization of axial histidines in bacterial reaction centers balances the asymmetry of the special pair"
A. Alia, P.K. Wawrzyniak, G.J. Janssen, F. Buda, J. Matysik, H.J.M. de Groot
J. Am. Chem. Soc., 2009, 131, 9626–9627

"Zinc chlorins for artificial light-harvesting, self-assemble into antiparallel stacks forming a microcrystalline solid-state material"
S. Ganapathy, S. Sengupta, P.K. Wawrzyniak, V. Huber, F. Buda, U. Baumeister, F. Würthner, H.J.M. de Groot
Proc. Natl. Acad. Sci. USA, 2009, 106, 11472–11477

"Alternating syn-anti bacteriochlorophylls form concentric helical nanotubes in chlorosomes"
S. Ganapathy, G.T. Oostergetel, P.K. Wawrzyniak, M. Reus, A. Gomez Maqueo Chew, F. Buda, E.J. Boekema, D.A. Bryant, A.R. Holzwarth, H.J.M. de Groot
Proc. Natl. Acad. Sci. USA, 2009, 106, 8525–8530

"Protein-induced geometric constraints and charge transfer in bacteriochlorophyll-histidine complexes in LH2"
P.K. Wawrzyniak, A. Alia, R.G. Schaap, M.M. Heemskerk, H.J.M. de Groot, F. Buda
Phys. Chem. Chem. Phys., 2008, 10, 6971–6978

"Electronic structure of axial histidines in photosynthetic reaction centres of Rhodobacter sphaeroides"
A. Alia, P.K. Wawrzyniak, F. Buda, J. Matysik, H.J.M. de Groot
Photosynth. Res., 2007, 91, 146–147 (Proceedings of the 14^{th} International Congress of Photosynthesis, Glasgow, UK, July 2007)

"Interaction energy decomposition analysis for formic acid complexes with argon and krypton atoms"
J.J. Panek, P.K. Wawrzyniak, Z. Latajka, J. Lundell
Chem. Phys. Lett., 2006, 417, 100–104

"Molecular simulations of formic acid"
J. Lundell, S. Jolkkonen, M. Saarelainen, P.K. Wawrzyniak, J. Panek, Z. Latajka

CSC Report on Scientific Computing in Finland 2004–2005, Fagerholm, Puska, Åström, Blomqvist, Forsström, Jukka, Kotila, Laine, Miettinen, Tarus and Tissari (Eds.); CSC, 2005, pp. 101–105
ISBN: 952-5520-04-8 (Print), 952-5520-05-6 (PDF)

"On the nature of bonding in HCOOH...Ar and HCOOH...Kr complexes"
P.K. Wawrzyniak, J. Panek, J. Lundell, Z. Latajka
J. Mol. Model., 2005, 11, 351–361

"Theoretical study of the complex between formic acid and argon"
P.K. Wawrzyniak, J. Panek, Z. Latajka, J. Lundell
J. Mol. Struct., 2004, 691, 115–122 and J. Mol. Struct., 2004, 704, 297–304