A computational study of structural and excitonic properties of chlorosomes

Li, X.

List of publications

Main Publications

- **Xinmeng Li**, Francesco Buda, Huub J.M. de Groot, and G. J. Agur Sevink, Contrasting Modes of Self-Assembly and Hydrogen-Bonding Heterogeneity in Chlorosomes of *Chlorobaculum tepidum*, *J. Phys. Chem. C*, **2018**, 122, 14877–14888. DOI: 10.1021/acs.jpcc.8b01790 (**Chapter** 2).
- **Xinmeng Li**, Francesco Buda, Huub J.M. de Groot, and G. J. Agur Sevink, Molecular Insight in the Optical Response of Tubular Chlorosomal Assemblies, J. Phys. Chem. C, **2019**, 123, 16462–16478. DOI: 10.1021/acs.jpcc.9b03913 (**Chapter** 3).
- **Xinmeng Li**, Francesco Buda, Huub J.M. de Groot, and G. J. Agur Sevink, Dynamic Disorder Drives Exciton Transfer in Tubular Chlorosomal Assemblies, **2020**, *submitted* (**Chapter** 4).
- **Xinmeng Li**, Francesco Buda, Huub J.M. de Groot, and G. J. Agur Sevink, *In Silico* Prediction of Chirality versus Optical Responses of Chlorosomal Tube Aggregates, **2020**, *to be submitted* (**Chapter** 5).

§ ***Code.*** A software package "CTubeGen" that generates atomistic tube structure of chlorosomes.(https://doi.org/10.5281/zenodo.3677028)

The following is a list of additional publications not included in the thesis.

- Xiaonan Kan,Chengyi Xiao,**Xinmeng Li**, Bin Su, Yuchen Wu, Wei Jiang, Zhaohui Wang, Lei Jiang, A Dewetting-Induced Assembly Strategy for Precisely Patterning Organic Single Crystals in OFETs, ACS Appl. Mater. Interfaces, **2016**, 8,18978-18984. DOI: 10.1021/acsami.6b04163
- Xiansha Xiao, Joost Willemse, Patrick Voskamp, **Xinmeng Li**, Meindert Lamers, Jan Pieter Abrahams, Navraj Pannu, Gilles P. van Wezel, Longitudinal cell division is associated with single mutations in the FtsZ-recruiting SsgB in Streptomyces, **2019**, bioRxiv 860916. Doi: https://doi.org/10.1101/860916

Curriculum Vitae

The author, Xinmeng Li, was born on the 11th of May 1990 in Binzhou, Shandong Province, China. He grew up in a village in Wudi county, belonging to an alluvial plain and near the Bohai Sea, flat everywhere, except around ten kilometers from where he lives, there is a hill, originally named as “giant mountain”, which is 63.4 meters high and covers an area of 0.39 square kilometers.

In 2007, he went to Harbin city in the most northeast province in China, Heilongjiang, and enrolled in the Northeast Forestry University to study polymer material science, developed interests in theoretical/numerical methods, and received a bachelor degree in 2011. Successively, he went to the Institute of Chemistry Chinese Academy of Sciences in Beijing to perform computational research under the supervision of Prof. H. Guo, where he explored multi-scale MD simulation methods, and received a master degree in in Polymer Physics and Chemistry in 2015. In September 2015, he moved to Leiden, the Netherlands, and started his PhD research under the supervision of Dr. Agur Sevink and Prof. dr. Huub de Groot at Leiden Institute of Chemistry, Leiden University. During his PhD research about chlorosomes, he extended his research skills to linear optical spectra simulation, diffraction prediction of helical structures and quantum dynamics simulation. He also developed a helical tube reconstruction software. He gave oral presentations of his work at Physics Veldhoven (Jan. 2017), CHAINS (Dec. 2017), Dutch Molecular Dynamics Day (Mar. 2018), Summer School Multi-Scale Modeling at Lorentz Center (Jun. 2019), and Han-sur-Lesse Winter school on Theoretical Chemistry and Spectroscopy (Dec. 2016 and Dec. 2018). He also started to cycle. He cycled with Agur Sevink many times in Netherlands including once around the IJsselmeer (lake) passing the Afsluitdijk, and twice the Dam tot Dam FietsClassic events. He also has cycled along the Pieterpad from Sint-Pietersberg (Maastricht) to Pieterburen (Groningen) in Netherlands (summer 2016), from Han-sur-Lesse to Leuven in Belgium (winter 2018), and along Rhine river from Basel Switzerland to Rotterdam Netherlands (summer 2019).

Afterword

At the end of the thesis, I felt that I have gone through a wonderful adventure. To reach this point, I have made a lot of effort, and I want to emphasize here that some insights originated from daily life activities also contributed. As you may have found, the thesis has a strong focus on one unique degree of freedom, *i.e.* head-head twisting/rotational motions. This focus is largely inspired by the simple idea that a book (plate) spins easily on a finger (stick), after noticing that similarly the heads of BChl pigments in chlorosomes are supported by thin Mg-O coordination bonds (Figure 1.6). It is my luck that I can work it out. Below, I express my gratitude.

The author is spinning a book on his finger.

First, I would like to express my sincere gratitude to Huub de Groot, Francesco Buda, and Agur Sevink for making this happen. The picture of you three during my skype job interview in the summer of 2015 is still vivid. Since then, it has been a wonderful experience for me working with you together in Leiden. Huub, as my promotor, I am grateful for all your input and high scientific standard, which make this research a better one. I didn't become world-famous as you mentioned, but I still feel happy that you enjoy the outcome of this research, and thank you for all your encouragement. Franco, it is great to have you with your kindness, expertise, and wisdom. I always find comfort and benefit each time after a discussion with you. Thank you so much. Agur, as my supervisor, I owe you the most. Actively, you make sure that things went correct; passively, you share the joy (new finding! new figures!) and upsets (not possible! ridiculous, how could they do this!). You have been a great supervisor and a great friend to me;

thank you for always being there and for giving me your invaluable support, guidance, and help. Also, thank you, Soraya, for always treating me well (the beer caddy you gave to me is excellent).

Next, my gratitude to all the members in our BPOC/SSNMR group for being friendly, supportive, and warm-hearted. Especially for my office mates, and for who were visited/bothered by me, as I like to walk around when I solved something. Alia, Anjali, Brijith, Chen, Dario, Dieuwertje, Emanuela, Faezeh, Fatameh, Fons, Jan Paul, Jessica, Karthick, Kiran, Laura, Liesbeth, Lijin, Lina, Lolita, Maithili, Remco, Rianne, Rico, Rubin, Srividya(Vidya), Tirong, Yang, Yuliya, and Zhongwu, as well as other people I met in the university, thank you all. Especially, Liesbeth, thank you for always being there and taking care of all the problems I bring to you. I hope the trick I was walking with a USB mouse pet can bring you some amusement. It is also fantastic for me to meet some Chinese friends in this lovely city. Although we may not be able to meet here anymore, 青山一道同云雨, 明月何曾是两乡.

I am also grateful for the members of the reading committee. Thank you for all your effort and time in the reading and assessment of my thesis. I would like to express my gratitude to all the people giving me understanding, support, and help during my graduation procedure, especially during such a hard time with the outbreak of COVID-19.

My special gratitude goes towards QQ. Thank you for bringing color and sound into my silent film life. The moment you were cooking swimming crab and I was writing on a tissue calculating the distances between helices is one of what I most cherished. Last but not least, my heartfelt gratitude towards my parents and other family members for their patience and support all the time.

Xinmeng
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