ACKNOWLEDGEMENTS

First of all I would like to thank my supervisor Prof. Ernst-Walter Knapp, for giving me an opportunity to work in his group. I am deeply grateful to him for creation of a nice working atmosphere, his permanent assistance, useful advices, plenty of helpful discussions leading to new ideas, and for supporting me a lot by solving the every-day problems.

I would like to thank Dr. Marcel Schmidt am Busch for introducing me to the computational methods and for the useful discussions.

I wish to acknowledge Prof. Snezana Zarić for her collaboration in my first quantumchemical project related to heme and Dr. Hiroshi Ishikita for collaboration in the projects related to the bacterial photosynthetic reaction center.

I am grateful to Björn Kolbeck, for introducing me to the administration of our Computer-Cluster. My thanks to Henning Riedesel and Florian Krull for helping me to keep computers running.

I would like to thank the Deutsche Forschungsgemeinschaft (Sfb 498 Project A5, GRK 80/2; GRK 268; GRK 788/1) for the financial support and Dr. D. Bashford and Dr. M. Karplus for providing the programs MEAD and CHARMM, respectively.

Finally I would like to thank all members of our group for the warm and kind atmosphere and for their constant readiness to help.