Quantum chemical studies of the physics around the metal-insulator transition in (EDO-TTF)2PF6
Linker, Gerrit-Jan

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2016

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):

Copyright
Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Download date: 07-07-2019
This work started after a meeting with Ria Broer shortly after Christmas 2007. Ria introduced me to the EDO-TTF material on which Daniele Fausti, a former PhD student of Paul van Loosdrecht, had performed Raman measurements. Ria and I agreed to perform calculations on this material and see where the project would take us. I had not been involved with chemistry since my graduation in 1995. My learning curve therefore was quite steep in January 2008 when I started reading a quantum chemistry text book that Ria recommended as a good read. In order to do the scientific work I arranged to work a day less as a freelance programmer. In April 2008, discussions started with Piet van Duijnen. His DRF model seemed perfect to predict the interactions between charged and neutral molecules. Thursday became my regular day at the lab, which it still is. At the lab, I initially shared office with Aymeric Sadoc, and later with Rob Klooster. Other PhD students in the group at that time were Adrian Stan, Reshmi Kurian, and Muizz Pradipto. I would like to thank you all for allowing me a gentle return into academia and for making me feel so welcome. I thank Daniele for the initial discussions on the subject, which I enjoyed very much.

It was Piet van Duijnen who persuaded me to convert the EDO-TTF research into a PhD project after publication of the first paper in 2010. Piet, I cannot thank you enough for all the time you have invested in me – for being at the lab for me every week. Thank you for all your support, for your supervision, for your patience, for sharing your bright ideas, and for everything you taught me. I would like to thank Ria Broer for allowing me to work again in the Theoretical Chemistry group. Thank you for all the opportunities that you have given me, and for everything you taught me over the years. I thank Paul van Loosdrecht for guidance and discussions – always with a smile and a joke. Thank you for sharing your knowledge of physics with me. The many discussions with Remco Havenith helped me enormously. It was especially important for me in the early years of the PhD project. Thank you Remco for the stimulating discussions, for everything I learned from you, for all your support and for always being there for advice.

It is nearly impossible to mention all other senior scientists, PhD colleagues and students I met and had inspiring discussions with. I especially wish to thank Wim Nieuwpoort, Coen de Graaf, Marcel Swart, Michael Filatov, Auke Meetsma, Ad van der Avoird, Robert de Groot, Iberio de P.R. Moreira, Evert Jan Baerends, Marina Servol, Fulvio Parmigiani for stimulating scientific discussions. I thank current and past group members for the great atmosphere and working environment. A few people I would like to mention specifically. I thank Andranik Kazaryan and Hilde de Gier for giving me the honour to be paranymph at their thesis defence ceremony. Andranik, I especially recall the evening we discussed your thesis and when your wife cooked a delicious dinner for us. Those discussions in 2010 were very stimulating for me. I am also very grateful that you are now supporting me as a paranymph. Hilde, it was very nice to be PhD buddies and to attend the many schools and conferences together, including: Han sur Lesse, Veldhoven, Groningen, Sicily, and Texel. I also enjoyed our discussions, especially our studies of ‘the open shell case’ springs to mind. I thank Muizz Pradipto, Remi Maurice, Naureen Akhtar, and Andrii Rudavskyi, for the motivating discussions, being scientific or on other subjects. I also wish to thank Johan Heijnen for giving technical support, and I would like to thank Henriet van Mil-Boddeveld and Jeannette de Boer for secretarial support.
Maartje, ik wil je bedanken dat je me altijd hebt gesteund in het doen van dit interessante werk. Er zijn zoveel andere dingen die ook gedaan moeten worden in ons drukke familieleven en ik hoop dat ik een beetje een redelijke balans heb kunnen vinden in dat alles. Arjan, Francien, Dirk en Renske ook jullie wil ik graag bedanken. Dat jullie lieve kinderen zijn natuurlijk, maar ook voor jullie interesse in alles om ons heen: de natuur, muziek, de dingen die ons leven mooi maken. Er is zoveel te ontdekken! Bedankt voor jullie mooie uitspraken waarop ik een aantal stellingen bij dit proefschrift kon formuleren. Een speciale vermelding wil ik graag maken voor mijn oma, Joke Japenga Veenstra. Het laatste jaar kwam ik vaak even bij je langs op donderdagavond, na een lange dag op het lab. Fijn dat je altijd interesse hebt getoond.

I also thank my parents and other family and friends for showing an interest in my work over the years. I especially thank Vincent Frucuoso van der Veen for all the discussions about your work and your interest in my work. I enjoyed it very much to have been involved in the presentation your poster and book at physics@FOM. Thank you for assisting me as a paranymph at my thesis defence.

Finally, I would like to mention T. Hoogewerf, a former pedel of our university, and family member. My grandmother recalled that the cousin of her grandfather used to be pedel in our university in Groningen. And memory served her well! With the help of Liza van Eijck of the office of the university, the university museum, and the current pedel, we found out that T. Hoogewerf was the last traditional pedel from 1957 until 1977.

Gerrit-Jan Linker