Competence-Based, Research-Related Lab Courses for Materials Modeling: The Case of Organic Photovoltaics

Karl Sebastian Schellhammer* and Gianaurelio Cuniberti

Institute for Materials Science, Dresden Center for Computational Materials Science and Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

Supporting Information

ABSTRACT: We are hereby presenting a didactic concept for an advanced lab course that focuses on the design of donor materials for organic solar cells. Its research-related and competence-based approach qualifies the students to independently and creatively apply computational methods and to profoundly and critically discuss the results obtained. The high degree of multidisciplinarity and the diversity of both the field of materials modeling and the students are considered within a modularized structure that allows the students to advance according to their individual abilities and interests. On the basis of our experience, through a hands-on format, it is possible to effectively capture the students’ intrinsic interest in this research field and prepare them for their future work in academia and industry.

KEYWORDS: Graduate Education/Research, Organic Chemistry, Interdisciplinary/Multidisciplinary, Physical Chemistry, Collaborative/Cooperative Learning, Computer-Based Learning, Inquiry-Based/Discovery Learning, Applications of Chemistry, Molecular Modeling

INTRODUCTION

Organic solar cells (OSCs) based on small molecules are potential candidates for low-cost large-area photovoltaic applications as they can be produced on flexible substrates, with little material consumption, and at ambient conditions. However, in order to further improve the device’s efficiency, development of new materials is essential. Given the high amount of possible functionalization routes, the potential complexity of synthesis, and the strong correlation between molecular structure and macroscopic material behavior, a theoretical preselection of molecular characteristics is needed. Furthermore, theoretical investigation can help to establish a deep understanding of organic chemistry and experimental observations, which is the basis for the formulation of universal design rules.

The importance of molecular modeling techniques for chemical education has been highlighted already by other educators, and the three-dimensional visualization of molecular materials is known to propel the learning process of students. However, it often occurs that lab courses are mostly based on an educational perspective, without any relevance for current research due to limited computer power, or because they require a connection to a supercomputer.

We therefore present a lab course for Master students focusing on the structure–property relationships of small-molecule donor materials for application in OSCs. By using a modularized structure with students working in small multidisciplinary groups on different yet overlapping tasks, they are trained in both simulation techniques for molecular materials and competences of scientific work. The lab course aims at qualifying and engaging students to independently and creatively apply the techniques to new research objectives, critically discuss the results obtained in a multidisciplinary context, and present them in terms of scientific publications. The computational methods combine both reliability and scalability providing the opportunity to experimentally extract relevant quantities already at desktop machines.

PREPARATION FOR THE LAB COURSE

The lab course is embedded in the lecture series Concepts of Molecular Modeling at TU Dresden, which consists of a weekly lecture and a hands-on seminar with a length of 90 min each. Approximately 50 students take the course in the first semester of their Master studies, the majority of which have a Bachelor degree in physics, chemistry, biotechnology, or materials science. Due to the diverse curricula of the students, neither an advanced background in organic chemistry nor in quantum chemistry can be expected for a minimum of one-third of the students. It is also worth mentioning that only a minority of them are trained in programming. Consequently, the first 2.5 months of the semester are used to prepare the students for the lab course.

Received: July 6, 2016
Revised: December 9, 2016
The lectures and seminars focus on intra- and intermolecular interactions, molecular orbitals, the Born–Oppenheimer approximation, the Verlet algorithm, the basics of thermodynamics and statistical mechanics, and the concept of normal modes (cf. Table S1 in the Supporting Information (SI)). In addition to this, during the seminars, students are trained in programming with SCILAB. Within the lab course, students are not required to write their own codes, but it is favorable for them to understand and manipulate the scripts they have been given rather than use them like a black box. Two weeks before the beginning of the lab course, the students have two hands-on sessions on the programs used within the lab course (see SI): MAESTRO for structure creation,17 VMD for visualization,18 density-functional-based tight-binding (DFTB) theory as implemented in the DFTB+ suite for simulation,19 and XMGRACE for data analysis. It is at this moment that they receive fully commented input files for material analysis using DFTB+ which strongly helps students to manipulate them independently during the lab course. Finally, it is important to mention that excellent tutorials and manuals for the above-mentioned programs can be found on the Internet and students are encouraged to work through such means as additional preparation for the lab course.

## ORGANIZATION OF THE LAB COURSE

The didactic concept was motivated by three pedagogical objectives:

1. The diversity of the students should be used for a multidisciplinary discussion and solution of a complex scientific problem. This is further promoted by the fact that only a few students meet all prerequisites necessary for such a demanding lab course. As a consequence of this factor, it becomes increasingly important for students to learn from each other’s experience and knowledge.

2. Despite already having a Bachelor degree, most students were not trained in competences needed for scientific work as well as for the preparation of their Master thesis. The lab course should therefore provide a first simulation of personal research activities including literature survey, data acquisition, analysis, and discussion, as well as publication.

3. Scientific work is based on compromises rather than clear solutions. A fundamental element of the lab course should include elements forcing students to find a balance between contrary aspects, e.g., simulation time and accuracy.

To reach such objectives, it was decided to make this lab course relatively open as the students need to analyze a materials class from different perspectives and propose their own molecule with optimized performance as donor material in OSCs. This task is split in four modules to account for the diversity of the students. As presented in Figure 1, each module focuses on different material characteristics that need to be considered for the design of improved donor materials, i.e., the electronic structure, the charge transport, the thermal stability, and the solubility. Such a concept allows the students to advance depending on their interests and background. In accordance with the modularized structure, the students work in groups of 3–4 people in which every member is free to select a different module. To maintain a realistic simulation of scientific work, it is preferable to form multidisciplinary, complementary teams. The results of the individual modules can be complementary but also oppositional motivating controversial group discussions as demonstrated in the SI.

At the end of the lab course, each group submits a project report in the spirit of a scientific publication limited to a maximum of 10 pages. Grading is not based on the number of molecules studied within the lab course, allowing students to adjust the workload within the lab course to their interests and obligations. Most focus is put on the reliability of the discussion including the weighting of multiple aspects for the design of donor materials, the critical discussion of the methods applied, or the comparison with literature data.

Students’ working time may vary from 80 to 120 h, distributed over 9 weeks from the introduction of the lab course to the submission of the final report. In the first 6 weeks, students are provided didactic support via weekly consultation slots as presented in Figure 2. One week before the lab course officially starts (with the first hands-on session on simulation techniques), students receive the descriptions of the modules and assign their first and second choices, which is an essential criterion for setting up the groups. During the introduction class, the working principle of OSCs is explained and discussed in detail, further motivating the individual tasks of the lab course.
The groups are announced, and time is given for questions concerning the groups and the tasks of the lab course.

In the following 2 weeks, consultations are organized mostly as open question and answer (Q&A) sessions. In this situation, students are individually working on their problems while questions are discussed simultaneously at a personal level. However, if specific questions or problems occur to multiple students, small input talks are included as well.

After 3 weeks, there is a class of 60 min per module. At this stage, most students are very familiar with the methods and have obtained their first results. Therefore, it is helpful to present and discuss the results in a global picture and to motivate which will be the next steps of their work. This consultation also helps students to share experiences, results, and ideas improving the performance of each one of them. These sessions partly shift the Q&A session from the tutors to learning groups made by students themselves.

After 4 weeks of project work, most students have finished all the tasks of their module for a minimum of three molecules and display less reliance on the tutors concerning technical and scientific problems. Accordingly, a seminar introduces the students into the basics of scientific writing, including structures of publications, title and abstract formulation, citation, as well as data presentation and visualization. They are encouraged not to present all of their results like in standard lab protocols but to arrange them according to one consistent story. In the second part of the consultation, seminars of 20 min each are arranged with the individual groups to support the group work. Until now, students have mostly worked independently collaborating with colleagues taking the same module. Consequently, these seminars help to find an overlap between the work of each group member and to construct a story for the report. Again, it is most important to put the results of the group into a bigger picture, given the fact that many students tend to lose the focus on the main task of the project due to the high amount of data obtained.

The last official consultation is organized as an open Q&A session because students or entire groups face different problems especially concerning the preparation of the report. In most cases, students need four more weeks to finish and submit their reports. During this time, it is helpful to offer them the possibility to submit a test page for constructive feedback in scientific writing.

In addition to the weekly consultations, students receive regular newsletters which give updates to several problems, answer frequently asked questions, and provide protocols for the consultations. Furthermore, students can discuss problems via Facebook in chat groups as well as with the tutors. As the students can work on the tasks of the lab course almost anytime, it is helpful to support them similarly.

After two repetitions of the lab course organized following the presented format, this didactic concept has been shown to provide the best support for the students and has led to an excellent performance from their side. As the entire lab course is ambitious, it is important that the students start with their work within the first week of the lab course and distribute the workload over the given time. It is worth mentioning that students tend to work individually during the first weeks of the course. This leads to the investigation of different molecules by the members of a team which is disadvantageous. In contrast, good coordination of the work within the groups leads to reduced workload and improved reports.

From the technical side, a Linux-based PC pool is favorable. However, all software packages used are open-source or free of charge for teaching purposes, allowing students to use their private computers as well. If a supercomputer is available, simulation times could be reduced and software packages working at higher accuracy could be used. Notwithstanding, an improvement in the learning success by these changes is not expected. Some of the approaches used in the modules have clear weaknesses, and we believe that coping with these weaknesses as well as with a critical discussion of the results obtained are two essential competences needed for scientific work. Additionally, students creatively work on improvements of the computational methods and always need to find a balance between accuracy and computational effort.

### RESEARCH OBJECTIVES

The main task of the students is that of finding a new molecule of the class of 2-(2H-pyrrro1-2-ylidenemethyl)-1H-pyrole (dipyromethenes, DPMs) that shows a red-shifted absorption maximum and overall best performance for application as donor material.20 The choice of this particular materials class is motivated by recent theoretical studies and their expected similarity to the materials class of 4,4’-difluoro-4-bora-3a,4a-diaza-s-indacenes (BODIPYs).4,5,25 BODIPYs have gained increasing importance as strong infrared absorbers yielding power conversion efficiencies up to 4.5% in evaporated bulk heterojunction devices and 10.4% in triple OSCs.25 For these molecules, slight changes in the molecular structure can strongly affect the material properties and the device performance.4,5,24,25 However, Slater–Koster files needed to perform simulations with DFTB+ are not yet available for the boron-difluoride group. With the successful synthesis and application of fluorene-functionalized BODIPYs, application of the lab course to these materials appears possible.7 However, as such molecules are bigger than DPMs, simulation times would be further increased. Consequently, DPMs show a superior balance between size, structure-dependent properties, and applications making them a reasonable choice for the lab course.

To adapt the complexity to the given resources, the lab course addresses the energy levels of the molecules, the hole transport, the thermal stability, and the solubility of the molecules (see SI). These aspects are not only relevant for application of donor materials in OSCs but also for many other scientific fields which request material engineering to be conducted.

### CONCLUSIONS

On the basis of a multidisciplinary, research-related, and competence-based lab course implemented in the lecture series Concepts of Molecular Modeling at TU Dresden, students are qualified to independently and creatively apply computational methods for the design of donor materials for OSCs. Moreover, a working atmosphere is created, preparing students for their future research activities in academia and industry. Instead of working through a detailed guideline, neither giving consideration to their intellectual talents, nor giving freedom to advance in accord with their interests and talents, students work in small groups on complementary, relatively free modules for one global goal. This setup along with the didactic support empowers them to operate in this field which critically discuss science and motivates them to understand the research objectives as profoundly as possible.
Since the start of this lab course at the TU Dresden two years ago, we have witnessed a strong increase in the practical performance by the students and in the quality of the reports submitted to pass the lab course. Students show a deep understanding of the correlation between molecular properties and OSC performance, and know strategies to improve them by chemical functionalization. 95% of all students have completed the assignments in their entirety for at least three molecules. Already after 4 weeks, technical questions are minor, and 75% of the students display less reliance on the mentors. After the lab course, all students use the computational methods with ease, while being able to reliably manipulate the input files rather than using the codes as black boxes. More than 50% of the students demonstrate extraordinary initiative leading to the simulation and design of more than 10 molecules, the advancement of the applied simulation techniques, or the application of information from external sources to their own data analysis. Many students show strong collaboration with colleagues within their own group and within the module allowing them to analyze a larger data set in the report and to solve and discuss problems without contacting the tutors. The evaluation of the lecture series provided by the students has strongly improved, and it was they who requested a growing number of courses of this kind, as they clearly feel the benefits provided by the use of the didactic concept. Since the development of the lab course, students combine their experimental work during the Master thesis with the software used is open-source even allowing the students to calculate their calculations on standard Linux PC pools and learn only for this course!!!

At least it should be highlighted that the concept does not necessarily lead to a strong increase in human resources needed for the coordination of the lab course. In contrast, it will lead to highly motivated and engaged students who are well-prepared for further research activities. We would like to close with a quote by a student: “If I hadn’t other responsibilities I would learn only for this course!!!”

**ASSOCIATED CONTENT**

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.6b00499. Worksheets, information on the preparation for the lab course, content of the modules, and discussion of possible modifications for applying the lab course to undergraduate students (PDF, DOCX)

**AUTHOR INFORMATION**

*E-mail: sebastian.schellhammer@tu-dresden.de.*

**ORCID**

Karl Sebastian Schellhammer: 0000-0001-8418-6401
Gianauelio Cuniberti: 0000-0002-6574-7848

**Notes**

The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**

This work was financially supported by the Heinrich-Böll-Stiftung e.V. and the German Excellence Initiative via the Cluster of Excellence EXC 1056 “Center for Advancing Electronics Dresden” (cAED). Computational resources were provided by the Center for Information Services and High Performance Computing (ZIH) of Dresden University of Technology. The authors would like to thank the Hochschuldidaktisches Zentrum Sachsen (HDS) and Zentrum für Weiterbildung at TU Dresden for support and fruitful discussions and Eliana del Bianco for linguistic revision of the manuscript.

**REFERENCES**

(14) Rodrigues, R. P.; Andrade, S. F.; Mantoani, S. P.; Eifler-Lima, V. L.; Silva, V. B.; Kawano, D. F. Using Free Computational Resources


