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A Model for Materials Science in Physics and Chemistry Curricula and Research at a Primarily Undergraduate Institution

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ABSTRACT

Materials science skills and knowledge, as an addition to the traditional curricula for physics and chemistry students, can be highly valuable for transition to graduate study or other career paths in materials science. The chemistry and physics departments at Weber State University (WSU) are harnessing an interdisciplinary approach to materials science undergraduate research. These lecture and laboratory courses, and capstone experiences are, by design, complementary and can be taken independently of one another and avoid unnecessary overlap or repetition. Specifically, we have a senior level materials theory course and a separate materials characterization laboratory course in the physics department, and a new lecture/laboratory course in the chemistry department. The chemistry laboratory experience emphasizes synthesis, while the physics lab course is focused on characterization techniques. Interdisciplinary research projects are available for students in both departments at the introductory or senior level. Using perovskite materials for solar cells, WSU is providing a framework of different perspectives in materials: making materials, the micro- and macrostructure of materials, and the interplay between materials to create working electronic devices. Metal-halide perovskites, a cutting-edge technology in the solar industry, allow WSU to showcase that undergraduate research can be relevant and important. The perovskite materials are made in the chemistry department and characterized in the physics department. The students involved directly organize the collaborative exchange of samples and data, working together to design experiments building ownership over the project and its outcomes. We will discuss the suite of options available to WSU students, how we have designed these curricula and research, as well as some results from students who have gone through the programs.

INTRODUCTION

Materials science is an interdisciplinary topic relevant to a variety of applications. Technology development has produced rapid growth and change in our society. Technology is often advanced by materials science improvements with examples in electronics, energy, and ceramics. At Weber State University (WSU), we are using materials science courses and research in addition to our traditional chemistry and physics curricula to better prepare students for future pathways in graduate school and industry [1].

WSU is a primarily undergraduate institution and serves a diverse population of students including a particularly large fraction of first-generation college students and veterans. The college of science at WSU is focusing on developing and broadening environmental and sustainability based research and teaching as an example to our community.

The interdisciplinary materials science curricula and research program fulfills two complementary goals: presenting high-impact labs and research, and emphasizing areas where we can broaden student participation in environmental and sustainable research and courses on campus.

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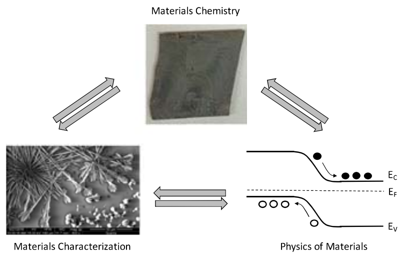

Figure 1. Interdisciplinary approach to materials science at WSU

CURRICULA

WSU has taken a collaborative approach to teaching its materials science courses. The materials science curricula at WSU include two survey style courses and one laboratory course. The survey courses include: *Physics of Materials* and *Materials Chemistry*. The laboratory course, *materials characterization lab*, is designed to utilize the foundational information gained in the survey courses. Figure 1 depicts the differences between the three courses. The *Materials Chemistry* course focuses on the synthesis of materials such as the perovskite, $CH_3NH_3PbI_3$, thin film shown above. The Materials Characterization course provides hands-on experience measuring structural, optical and electronic properties of materials such as that shown in the SEM picture. The course focuses on the fundamental physical properties of materials such as the band structure shown in the figure.

Materials Theory

The *Physics of Materials* course is designed as an introduction to the fundamental physical properties of solids and is broken into roughly four sections: static properties, dynamic properties, electronic properties, and applications. Each section also covers the appropriate experimental techniques needed to investigate the covered properties. The prerequisites for this course are Modern Physics, Thermal Physics, and College Chemistry.

The first section of the course (roughly four weeks), covers the static properties of materials, including bonding and structure. This includes structure of crystalline and amorphous materials. Students are also introduced to the theory of diffraction of waves from a material and experimental aspects of both x-ray diffraction and other diffraction methods.

The second section, dynamic properties of materials, covers lattice vibrations and heat capacities of materials, starting with the 1D classical monatomic lattice and continuing through phonons and a quantum model for heat capacity.

The third section, electronic properties of materials, covers Bloch functions, band theory, electrons in metals and in pure and doped semiconductors.

The fourth section highlights applications of solid materials including: semiconductor applications, nanostructures, and energy applications.

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The course uses traditional lectures and homework that is both traditional and makes use of computer simulations. Each of the sections of the course ended with a "journal club" reading and discussion of a current research article related to the topics covered. At the end of the course, students are required to present on a characterization method of their choice from a list provided by the instructor.

The course has consistently been one of the more popular elective courses in the department. Students have rated the course highly, giving an average rating of between 6 and 7 on a 1-7 scale. Students commented that the computer simulations were "helpful", and that the course was "practical" although "more theoretical than [they] had anticipated.

Materials Synthesis

The Materials Chemistry course is a survey course focusing on the synthesis of materials through gas, liquid, and solid phase reactions. While the prerequisites for this course are Foundations in Physical Chemistry and Foundations in Inorganic Chemistry, this course is designed to be complimentary to the Physics of Materials course offered in the physics department.

Both crystalline and molecular structures are studied with particular emphasis on how these parameters relate to electronic, optical, thermal, and mechanical properties. General synthetic considerations are covered including crystalline vs. amorphous growth, nucleation and growth mechanics of crystalline substances, and surface chemistry techniques. Beyond general synthetic strategies, highlights of current syntheses of attractive materials are discussed including syntheses for alloys and composites, glasses and ceramics, polymers, semiconductors, superconductors, nanomaterials, thin films, and porous materials. Current applications for materials are also discussed allowing students a view of the current availability of investigation after graduation from WSU.

The Materials Chemistry course also touches briefly on materials characterization including x-ray diffraction (XRD) and microscopy techniques. This brief introduction is designed to peak the interest of students towards taking the more in-depth materials characterization course offered in the physics department.

Materials Characterization

The Materials Characterization Lab is designed to give students the hands-on experience measuring structural, optical, and electronic properties of materials. Measurement techniques include: scanning electron microscopy (SEM), atomic force microscopy (AFM), x-ray diffraction (XRD), mechanical spectroscopy, and nuclear quadrapole resonance (NQR). Optical measurement techniques include: ultraviolet-visible spectroscopy (UV-VIS) and visible light diffraction. The students also gain experience in electronic device creation making dye-sensitized solar cells from blueberries similar to those made in Ref. [2]. The students also have the option to complete a final project using either our sputtering system or tube furnace to gain experience in thin-film growth. The materials characterization course uses the theory developed in the Physics of Materials and Materials Chemistry courses as student write final lab reports from selected labs. The students' lab notebooks are also graded according to a standard rubric.

This course was designed to use collaborative, team taught labs. As an example of a non-traditional team taught project, one of the labs features collaboration with our Microbiology

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department. In that lab, Materials Characterization students are paired with Microbial Physiology lab students. Bacteria cultures are made and prepped for study with SEM and AFM. With the new addition of the materials synthesis course, samples can be made by the chemistry department and prepped for study in a variety of our characterization tools.

The course is one of two options for a senior-level laboratory course in the physics department. Students have rated the course highly, giving an average rating of between 6 and 7 on a 1-7 scale. Student feedback was positive interns of the "variety" of experiments and equipment training. We are in the process of designing a survey instrument to test student perceptions of working across disciplinary boundaries after the collaborative exercise with the Microbial Physiology lab course.

Course Synergy

The Materials Synthesis course is the newest course to materials curricula at WSU. The course is specifically designed to dovetail with the other two courses while filling the knowledge gap of materials development. All three courses share a similar approach to student outcomes defining that students should be able to: 1) analyze crystalline and amorphous solid structure 2) predict and test physical properties of a material 3) critically evaluate current research.

The cornerstone of all three courses is understanding the structure of materials, however each course has a unique approach. The Materials Synthesis course approaches structure through molecular bonding. The Physics of Materials course approaches structure through atomic lattices. The Materials Characterization Lab takes an experimental approach of determining the actual structure of materials. Developing the courses this way helps the student understand that different disciplines and fields can study the same problem with a different type of insight bringing new knowledge and creative solutions.

All three courses include a final project and presentation. The final project for each course requires the student to complete a literature search and/or experiments on a specific material or characterization technique not covered in the course. The Materials Synthesis course requires students to research and present a specific material and corresponding synthetic technique not covered in class. The Physics of Materials course requires students to research present a specific material characterization technique not covered in the course. The Materials Characterization Lab requires each group to design their own experiment (or series of experiments) for the last two weeks of the semester.

Several times during the semester for both the Materials Chemistry and Physics of Materials courses, students are asked to read, analyze, and present on a recent journal article from a current topic in materials. Examples of these topics include but are not limited to: solar cells, nanostructures, characterization techniques, and liquid crystals. The students use these presentations to highlight their understanding of fundamental materials principles covered in the courses as well as to learn to evaluate current research.

RESEARCH

WSU has not only designed materials curricula to enhance our undergraduate experience in the physics and chemistry programs, but is also actively developing an interdisciplinary approach to materials science research.

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A major strategy for recruitment and retention of under-represented/first-generation students is to steer them to involvement in high-impact opportunities, like undergraduate research, that have been shown to help with retention of these students [3]. Thus, this expansion of undergraduate research opportunities for students interested in physics, chemistry and materials science complements an existing major university initiative for retention of underrepresented and first-generation students.

The first interdisciplinary project is the deposition and optimization of perovskite materials for solar cells. This project embodies the sustainability and environmental initiatives of the college of science while fulfilling the high-impact requirement needed to retain students.

Perovskites

Plastic solar cells have been utilized to help connect chemical concepts to active research in a multidisciplinary fashion [4]. Creation of solar photoelectrolysis materials have also been shown to effectively provide an interdisciplinary environment for students to learn [5]. Similarly to these projects, we are using solar cells to help connect both physical and chemical properties of materials to cutting-edge research to highlight the interdisciplinary nature of materials science. Perovskite materials have been an exciting addition to the solar materials community since 2009 [6]. Perovskites debuted in 2009 with 3.1% [7] efficiency and rose quickly to a current best laboratory cell efficiency of 22.1% [8]. The highest efficiency perovskites are inorganic/organic hybrid material compounds, $CH_3NH_3PbI_3$.

Perovskite materials can be deposited through a variety of methods, several of which are inexpensive and easily obtainable in an undergraduate laboratory [9]. Undergraduate chemistry students deposit the perovskite materials in one of our chemistry laboratories. Once the material has been deposited, the students bring the samples to the physics department for characterization. The students involved in this project were juniors and seniors who had already had some background in characterization and deposition.

Sample Synthesis

Chemistry undergraduate students began learning about materials deposition methods using a spin-coater (Figure 2). Spin-coating is an ideal starting point for learning materials synthesis as it is inexpensive, and easy to begin operating. Additionally, there are many parameters for optimization, allowing students to really explore how factors such as solution temperature, spin speed, spinning duration, and sample amount can all affect the resulting thin-film.

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Figure 2. Spin-coating PbI_2

The construction of perovskite materials begins with the deposition of PbI_2 on a glass substrate [10]. The PbI_2 solution is brightly colored and allowed students to quickly observe macroscopically the quality of the film. Initial attempts didn't even require microstructure analysis, as the macroscopic structure was still poor, including incomplete coverage across the substrate and the formation of rings within the film. Students found that both of these issues could be fixed by heating the initial solution, and spinning for a longer period of time. After initial optimization, fine-tuning of the deposition was performed based on the microstructure analysis provided by physics undergraduate students.

The second step for the perovskite layer is the inclusion of the methylamoniumiodide (CH_3NH_3I) component. Initially, this step has been accomplished via a dipping method with subsequent drying [10]. As seen in Figure 3, this changes the color of the film from a bright yellow to a dark grey/brown color indicating to the students that they have changed the materials structure and the resulting light absorption properties. The bandgap of the material was investigated by physics undergraduate students in order to determine what synthetic parameters to change, including film thickness, heating times, and concentration of the CH_3NH_3I solution. While the dipping method is a good starting point for our students, we are currently exploring a chemical vapor deposition method for increased performance of the material and to expose students to another deposition method [11].

(a) (b)

Figure 3. Two step method for creating $PbCH_3NH_3I_3$ solar cell materials at WSU (a) Spin-coated PbI_2 deposition by chemistry department, (b) CH_3NH_3I inclusion by dipping method by chemistry department.

The total construction of the solar cell includes a spin coating deposition of a TiO_2 electron transport layer and a Spiro-MeTAD hole transport layer. Finally, a conductive metal is thermally evaporated as a back contact [10]. The complete assembly, as seen in Figure 4, can

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then be investigated for photovoltaic properties. We are currently in the process of constructing a full cell.

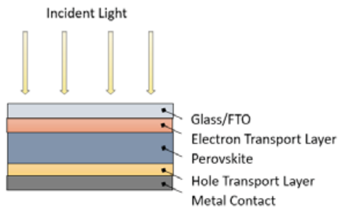
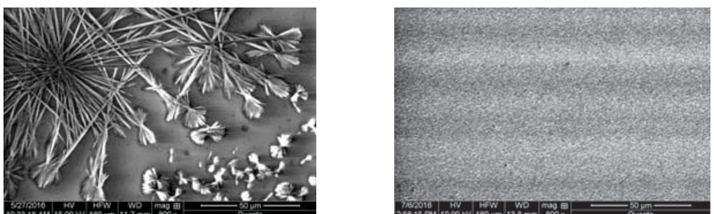


Figure 4. Schematic illustration of the components of a working perovskite-based solar cell being developed at WSU

Sample Characterization

Studying the microstructure of the material via SEM is the first step to analyzing the sample microstructure. Figure 5a shows an example of the microstructure of one of the first PbI_2 films deposited at WSU. Using energy dispersive X-ray spectroscopy (EDS), our physics undergraduate was able to determine that the sample had large PbI_2 crystals which is not optimal. Feeding this type of information back to the chemistry department, our chemistry undergraduate was able to adjust the deposition parameters necessary to achieve a more uniform microstructure as shown in Figure 5b.



(a) (b)

Figure 5. SEM images of PbI_2 films taken by students at WSU. (a) first PbI_2 film, (b) later PbI_2 film with improved microstructure.

Once a better microstructure was achieved, our physics undergraduate would measure the thickness of the film using AFM. Figure 6 shows the AFM image of one of our samples. The perovskite films are soft and can be scratched easily to the glass slide using a sharp instrument. The scratched material will collect on the edge of the scratch, so thickness measurements were made using the two regions shown in the black circles. This sample had a thickness of

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approximately 400 nm. The calculated thicknesses are fed back to the chemistry department as information for refining and understanding the deposition process.

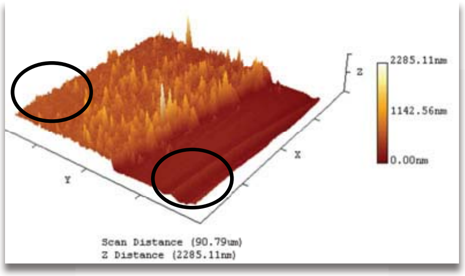

Figure 6. AFM image to measure material thickness taken by student at WSU

Once an optimal microstructure and thickness was obtained, our physics undergraduate was able to measure the bandgap energy of the material using UV-VIS. The undergraduate collected data and plotted the transmission of the light through the sample compared to the substrate. The transmission data was used to calculate the absorption coefficient and a Tauc plot was created as shown in Figure 7 using a method similar to that described in Ref. [12]. A linear fit is drawn through the linear region of the plot as shown by the black dotted line. The intersection with x-axis gives an estimate of the bandgap energy of the perovskite material. This particular sample has a bandgap of approximately 1.9 eV. The optimal bandgap for single junction solar cell is approximately 1.4 eV [13] so while not optimized, this particular sample was better than first attempts at the material.

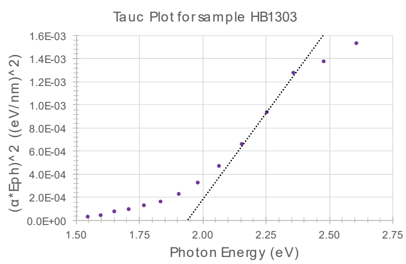

Figure 7. Example of bandgap energy analysis completed by student at WSU

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Solar Cell Device

While research grade electron and hole transport layer material recipes are being developed, the first solar cell device at WSU was created combining perovskite research with device processing covered in the Materials Characterization Lab course. Two undergraduates from our lab course were able to take the perovskite material made by the chemistry department and use the electron/hole transport structure used to make raspberry/blackberry based solar cells in class. Using the same methods as in class, the short circuit current and open circuit voltage were measured by the students.

Data Management

An iterative process was used for perovskite development at WSU (Figure 8). This process is unique opportunities for the students to learn soft skills such as team work, collaboration, organization, data management, and reporting. As samples were developed by chemistry students, they were analyzed by physics students and that information was in turn used to refine future samples.

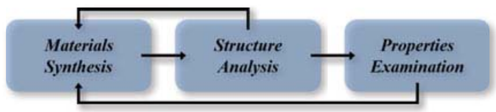

Figure 8. Material development feedback loop employed by physics and chemistry research teams at WSU

As part of the process, a large interactive spreadsheet was developed that each team member could access. This spreadsheet included sample number, all deposition parameters, two thumbnail images of the microstructure and sample, thickness information, and bandgap information. This document is accessible from a central location so that any information that is updated can be seen by the team.

This document helps students understand design of experiments and the importance of changing only one parameter at a time. It also helps communication among the group while teaching organization of experimental information especially when an experiment is repeated many times. This type of organizational document is also similar to that kept in industrial environments as materials recipes are developed.

CONCLUSIONS

Both of the physics and chemistry departments have reaped the benefits of the materials science program at WSU with respect to both faculty and students. Student interest has increased in both departments and multiple students are actively participating in the interdisciplinary research through the perovskite solar cell project. Past evidence has shown that this program is a pathway to graduate programs and industrial positions as several students have followed these paths in materials science following WSU. The interdisciplinary nature of the work is also more competitive for internal funding for both faculty and student research at WSU.

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This work has also brought new capabilities to our university opening the door for real electronic device research and exposure in courses. Overall, the addition of the materials science courses to our programs has been advantageous in a variety of ways to WSU.

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