Introduction

Translator Profile

- I work as an **independent consultant with my own private consulting company Property Vectors** focused on atomic-scale materials and chemistry modeling in a wide variety of application areas and HPC consulting. I previously worked as a Senior Research Scientist in the semiconductor industry effectively as an internal consultant to the experimental research and development teams.
- My **primary experience in materials modeling is focused on atomistic models with a particular focus on Plane Wave and Local Orbital Density Functional Theory**. I also have a significant amount of experience in classical Molecular Dynamics and less in Monte Carlo in the atomistic regime. Above the atomistic regime I have limited experience in Finite Element Modeling as well as a number of electrical resistance, device, and circuit models that are typical in the semiconductor field and well as three-dimensional process modeling. I have worked on a wide variety of mechanical (elastic constants, cohesive energy, stress vs. strain, CTE, and more) and electrical properties (static [resistivity, charge density, polarizability, dielectric constant, and Schottky Barrier] and dynamic [current density, IV])

Client

- In the past my "**clients**" were experimental co-workers in semiconductors working to research, qualify, and perfect new materials, chemistries, and then integrates structures in logic devices. My most recent customer in consulting is a defence contractor bidding with the government building a new Infrared camera that operates at a higher temperature through use of new materials technology. The defence contractor qualifies as a small business of less than 200 people.
- Both the large semiconductor company and the defence contractor qualify as **manufacturing companies** that perform their research and development in-house.
- I had a **prior relationship** with the defence contractor as they had offered me a full-time job in the past. In the case of the semiconductor company, I worked there for 15 years after starting as an intern after completing my Master's at Stanford and being recommended for the internship by my thesis advisor.

Industrial/Business Case

- In semiconductors, the **business case** is that the industry is predicated on Moore's Law and shrinking of the dimensions of a logic semiconductor chip to deliver an increase in computing power over time. These devices are the foundation that have helped drive the computing revolution of the past decades. This drive to reduce dimensions leads to changes in the current and power required in the chip and also in the thermal stresses. This leads to changing material property requirements that either require changing the structure or makeup of the original material or finding an entirely new material that meets the new property requirements. The crux of the problem in semiconductors however is usually that although you may be able to find a new material that meets the property requirements, it is extremely challenging to integrate it into the traditional semiconductor flow. This flow requires many different steps, chemistries, temperatures, and other materials that the new material will come into contact. In addition, the allowed defect percentages required for

optimum performance are orders of magnitude lower than what can be simulated in DFT as manufacturing needs to be done at a very high-quality level.
In the case of the defence contractor, they are looking to set out to meet a request for a new device that is more portable, lasts longer, and requires less collateral to keep at the optimum temperature that is higher than the operating temperature for current devices for a wide variety of defence applications. The requirements on the defects levels are significantly lessened in the case of the defence application as the acceptable signal-to-noise ratio is much higher than in the case of semiconductors.

- The **total budget** to develop the next generation of logic processing chip is on the order of 10's of billions of dollars. The portion dedicated exclusively to materials-type of research is significantly smaller portion of that budget, likely on the order of $1/10^{th}$ of the total R&D cost. There are extremely high capital costs for all source materials and machines that are part of the manufacturing process and the price pressure for an optimum price of the final chip is strong. Due to this, many different logic processing chips must be manufactured side-by-side to an extremely high level of quality. If we associate the budgets of large TCAD departments as being reflective on the allocation of funds towards materials related problems it amounts to at least 10-100's of millions of dollars per year. That does not account for the experimental budgets dedicated to materials.
  In the case of the defence contract the complete budget for the entire defence contract is on the order of a few million dollars. Of this on the order of a few 100k dollars is dedicated to the search for the right materials with modelling to meet the needs if the cost of engineers and computing is taken into account.
- In semiconductors the **expected outcome of the translation process** is to help identify a new or optimized material that can survive the varied processing steps and be manufactured at a very low defect level.
  In the defence contractor, the expected outcome is much more easily attainable goal of providing insight for the experimentalists in their search for a new material to meet their needs. In addition, the level of quality and difficulty of integration into a product is much lower. Finally, part of the role of translation with both cases is to educate the experimentally focused client about the power and limitations of the techniques and how despite their inherent errors they can be used to guide research and development at reduced cost and timeline.

Translation to modelling solution

- I will focus on the defence contractor alone in this case as the **range of models used** in semiconductors was too wide for the space allotted. I primarily used plane wave density functional theory to demonstrate the effectiveness to predict properties of interest to the company (band gap, defect states, etc.). The focus in this first stage was to generate data to help in the justification for a follow-on defence contract submission proposal. At the same time, I was training one internal engineer on these methods. While I focused on generating results and content for the defence contract proposal the client's engineer was also familiarizing himself with DFT tools and methodologies under my guidance. For that reason, I started with very general and basic DFT models as I was walking the engineer through the basics of DFT at the time and did not want to overload him. Throughout the discussion I explained to him the problems of convergence testing, importance of thickness of slab models being tested, and impacts of surface orientation and reconstruction. At this stage the **level of accuracy** was not very critical and 10% was acceptable as part of the role was just to identify a trend to show that these properties in principal could be modulated. Unlike in semiconductors at this stage, choosing a recommendation that was likely to manufacturable and integratable was not a concern. In the future for follow-on studies I suggested explore Non-Equilibrium Green Function Methods to estimate transport as well as potentially Time-Dependent DFT methods. I recommended that in the future device-level models may be required and we would need to identify what property inputs would be needed as data for those parameterized models from the DFT results. At this stage, no experiments were performed and previously published literature was used as a validation check. Most of the primary **final decisions on structures and models** used were made by me as the primary engineer I was working on was not extremely knowledgeable in this area. His advice and input mostly focused on making sure we were working on the right materials set.

Client's benefits from the modelling

- The client **used the model results** to show competency to the reviewer of the grant proposal in both in-person presentations and the actual writing of the grant proposal. I was not present at the presentation, but the overall impression from the client was that the funding agency representatives were happy with the results. The final decision on the funding grant is pending. In addition, I also made a series of predictions of the total computing and human resources that would be required for a long-term plan of the grant moving onto the more advanced techniques and device models I mentioned above. I also surveyed available HPC cloud computing options to supplement their sub-par academic based supercomputer that was used for the initial calculations and estimated the costs and benefits of various engines.
- For the defence contractor, the **monetary benefits** have not yet been realized. For the semiconductor company, it is extremely difficult to quantify except to say that my total compensation averaged approximately $200k for a decade.

Evaluation of the translation case

- **Bottlenecks** included bringing the less experienced engineer up-to-speed on the techniques and their tricks and difficulty of use. In addition, the lack of sufficiently reliable computing resources also was a significant impediment to the efficiency of the process. In the case of the semiconductor client, a large portion of the difficulty was related to gaining the confidence of skeptical experimental clients in the methods and their efficacy. It is always also a challenge to get high quality and timely characterization data to build our structural models that are representative of reality. Often times the real structures also would require a model size that was too computationally expensive and smaller models would need to be used instead.