Quantum and Atomic Scale Materials Modeling in the Philippines: Status, Challenges, and Recommendations

Ryan Lacdao Arevalo*

Department of Physics, University of San Carlos, Talamban Campus, Nasipit, Talamban, Cebu City 6000, Philippines

*Author to whom correspondence should be addressed; email: ryanlarevalo@gmail.com

ABSTRACT

The computational materials modeling and simulation research landscape in the Philippines is explored to identify the problem areas and challenges faced by the experts in this field, thereby gaining insights for policy recommendations towards advancing this field in the country. The identified problem areas based on a survey administered to sixteen expert-respondents include the inadequate computational infrastructure, issues on funding, problems with students, administrative and teaching assignments, and lack of collaborations with the industry. Based on these results, policy recommendations were formulated, which include a proposed framework for an integrated computational and experimental approach in the national research and development agenda, enhancement of the national computing facility, amendment of the procurement law, dedicated funding for computational science, establishment of a junior research fellowship and an organized materials modeling community, and development of regional niches for computational materials science.

Keywords: Computational materials science; Materials modeling; Policy recommendations

INTRODUCTION

With the advent of supercomputers, computational modeling/simulation has evolved to be the third pillar of scientific inquiry alongside theory and experiment (Skuse, 2019). Its application in the field of materials science has been argued to be a key enabler of research and development (R&D), efficiency and innovation. It has been shown that such materials modeling technique has benefited the industry by reducing the R&D time and cost, promoting a more efficient and targeted experimentation, and enhancing decision making and performance optimization (Adamovic,

2018). The remarkable impact of materials modeling is evidenced by the exponential increase in the number of global publications per year (Payne, 2020), as illustrated by Fig. 1.
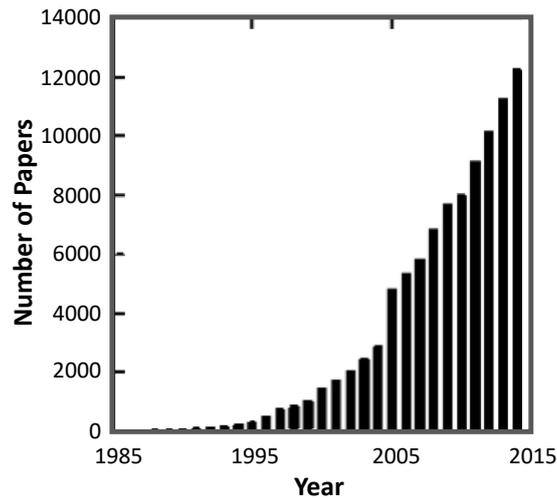

Figure 1: Representative number of global publications per year that utilized density functional theory (DFT). Adapted from Payne (2020) with permission.
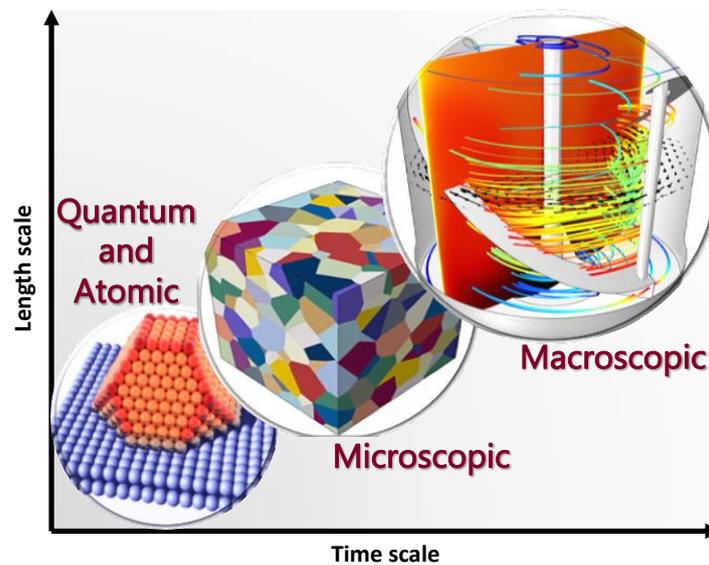

Figure 2: Multiscale materials modeling. The finer scale divisions within each of these overarching length and time scale regimes are not shown for simplicity.

Materials modeling has different methods and implementations that span a broad spectrum of length scale and time scale. A simplified multiscale materials modeling hierarchy is shown in Fig. 2, where three regions denoted as quantum and atomic, microscopic, and macroscopic scales are shown. The other finer scale divisions are not shown in the figure for simplicity. The quantum and atomic scale regimes are in the nm or less length scale, which span the level of the electrons, atoms, molecules, and nanomaterials. The microscopic regime is in the length scale greater than nm and up to mm. It encompasses microstructures such as grains, phases, sub-grain dislocation structures, point defects cluster, etc. (TMS, 2015). Modeling in the macroscopic regime involves systems with length scales greater than mm, which are implemented to study macroscopic properties such as mechanical, thermal, and structural design of materials. The focus of this paper is on the quantum and atomic scales of materials modeling.

In the quantum and atomistic scale modeling of materials, four principal modeling approaches are commonly used to serve as foundation for ab initio simulations. These include density functional theory (DFT), Quantum Monte Carlo (QMC) methods, classical potentials, and Ising models (TMS, 2015). The key statistical or micromechanical implementation methodologies of these modeling approaches include kinetic Monte Carlo (kMC), statistical Monte Carlo (sMC), molecular dynamics (MD), and phonon modeling. Recent interest in the use of artificial intelligence such as machine learning for materials simulation has also emerged for a high throughput screening and design of functional materials. These models and implementations have been widely used by computational materials scientists around the world to elucidate the atomic-scale mechanisms of chemical, biological, and industrial processes, and fundamental properties of nanomaterials for applications in catalysis, spintronics and electronics, materials design, among others.

Considering the role of materials modeling in innovation, it is imperative to integrate these methods in a wholistic materials science research agenda. To the best of our knowledge, while these methods are currently being used by a number of research groups in the Philippines, a national development program in materials modeling has never been proposed. Moreover, no study has been conducted on the extent of the use of these methods in materials science research among Filipino scientists. Such gap in the literature that elucidates the status and challenges of materials modeling in the Philippines can provide insights and bases for policies and development programs of the government for infrastructure, education, and research. The current study explores the state of quantum and atomic scale materials modeling in the Philippines, including gaps and limitations, and provides recommendations aimed at advancing this field in the country.

MATERIALS MODELING LANDSCAPE IN THE PHILIPPINES

Recent statistics has shown that the Philippines has about 189 scientists per million population from different fields of expertise, whereas the ideal ratio is 380 scientists per million population (Arayata, 2019). Aside from the fact that there is large gap between the ideal and actual ratios of scientists and the overall population, it is also unclear how many of these scientists are working in the field of quantum and atomic scale computational materials modeling and simulation. To this end, document analysis based on publications, institutional websites, and meeting reports was conducted to identify the experts in this field and the universities or research institutions where they are currently employed. An expert in such field is defined to be a full-time faculty or scientist in an institution who has either published at least one paper or conducted a graduate level research in the field of quantum and atomic scale materials modeling, and is capable of leading an independent research group in this field. All the identified experts were found to be employed exclusively in universities, indicating the lack of experts in the industry sector. Nine universities from different regions were identified to have at least one expert as shown in Table 1. It can be seen that most of these universities are concentrated in the National Capital Region (NCR), which can be attributed to several factors. First, the universities that offer graduate programs in physics, chemistry, and materials science are mostly located in the NCR. Second, the top Philippine universities identified by ranking agencies (such as the top 1000 universities by the QS World University Rankings and Times Higher Education World University Rankings) can also be found in the NCR, whose national academic reputation may have influenced the choice of workplace by the experts (Times World University Rankings, 2020; QS World University Rankings, 2020). Third, the faculty salaries and benefits in the NCR are generally higher than in the other regions (National Wages and Productivity Commission, 2020).

Table 1: Number of respondents per university and region.

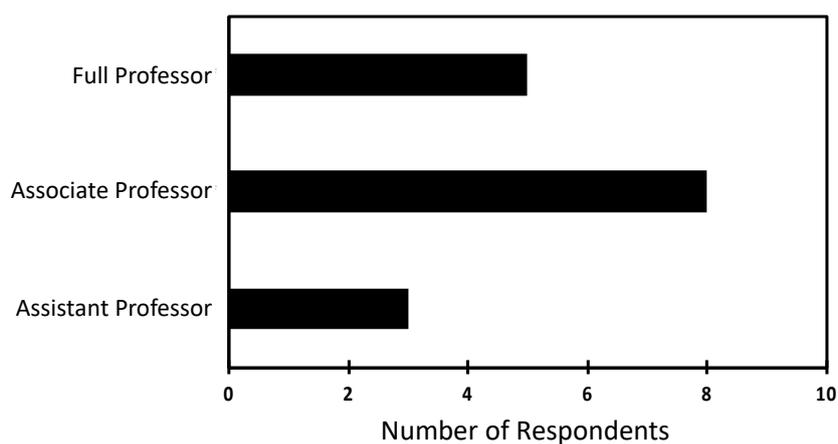| Region	University	No. of respondents
NCR	A	1
	B	2
	C	1
	D	1
	E	4
Luzon	F	4
	G	1
Visayas	H	1
Mindanao	I	1

Figure 3: The current academic ranks of respondents.

To evaluate the current status of computational materials modeling in the Philippines, survey forms were administered online to twenty-three identified experts in this field. However, only sixteen of these experts have submitted their responses. The number of respondents per university is presented in Table 1. As shown in Fig. 3, majority of these respondents are in the academic rank of associate professor level, which indicates that most of the experts in this field are in their mid-career stage. Also, 25% of the respondents are women. All of the respondents have a doctorate degree, except for one respondent in the assistant professor level who is currently taking up his doctorate. The countries where the respondents received their highest educational attainment are shown in Fig. 4. It can be noted that 69% of the respondents have received their highest educational degree abroad. Based on the survey, the specialization of the respondents in their highest educational degree are in the fields of computational materials science, theoretical condensed matter physics, computational chemistry, and molecular modeling in pharmaceutical science. Twelve out of sixteen respondents come from the corresponding Department of Physics of each university while only four respondents are from the Department of Chemistry. The number of students mentored by the respondents in different academic levels is shown in Fig. 5. This number includes all current and student graduates who were directly advised or co-advised by the respondents. It can be noted that most of the respondents have not experienced mentoring a doctoral student. Interestingly, the respondents who were able to mentor doctoral students come from all academic ranks, which indicates that advising doctoral students is not limited to those with a full professor rank. With regard to mentoring the bachelor's and master's students, majority of the respondents have only mentored 5 or less students in these academic levels. Such statistics indicates that there are generally few students who specialize in quantum and atomic scale materials modeling.
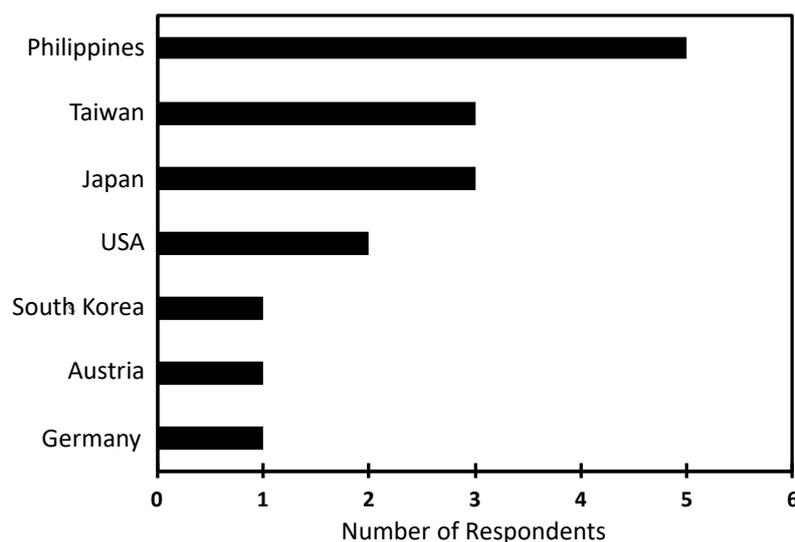
Figure 4: The countries where the respondents have received their highest educational degree.
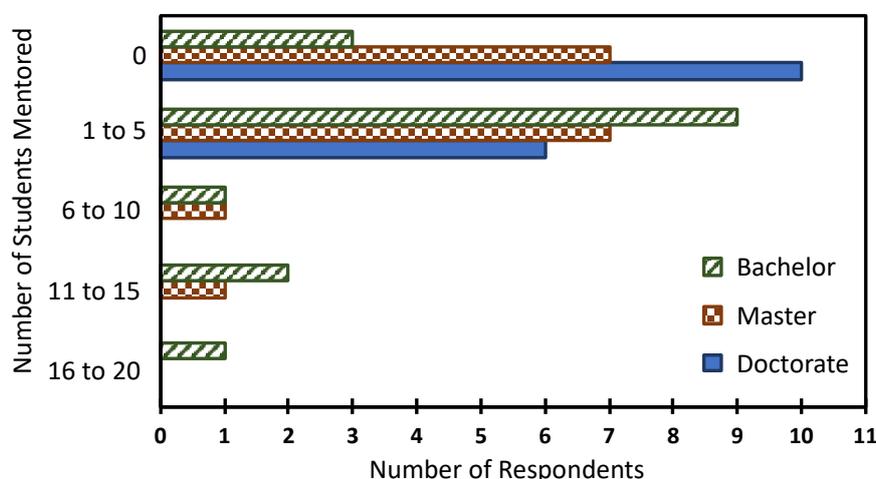

Figure 5: The number of students mentored in different academic levels by the respondents.

One important driver of research is the availability of grants that fund the acquisition of equipment, salary of researchers, and other pertinent expenses of the research group. Based on the survey, the respondents have received research grants from the national government agencies such as the Department of Science and Technology (DOST) and the Commission on Higher Education (CHED), local institutions such as the University of the Philippines and Mindanao State University, and foreign agencies such as the United States Agency for International Development (USAID), Japan Society for the Promotion of Science (JSPS), Taiwan Ministry of Science and Technology, and the National Research Foundation of Korea. This indicates the diversity of available funding institutions that support the field of computational materials modeling. In the Philippines, the government agency with the highest funding for research is the DOST. For CY 2020 alone, the approved budget for DOST-Grants-in-Aid program amounts to about 2 billion Philippine Pesos (CY 2020, Approved Projects, 2020). However, document analysis shows that only 2 out of the 254 approved projects are in the field of computational materials science. These projects include a computer-aided drug design and DFT-based study of an anode material for sodium-ion batteries.

Another important aspect of research is the collaboration with other researchers. The survey showed that nine out of sixteen respondents have ongoing collaborations with other institutions

in the Philippines, while ten out of sixteen respondents have ongoing collaborations with foreign institutions in countries such as USA, Japan, Malaysia, Taiwan, Italy, China, and Kazakhstan. It was further found that six out of the eleven respondents who have received their highest educational degree abroad were able to maintain their collaboration with their foreign alma mater, which provides a post-graduation follow-up mentoring and linkage.
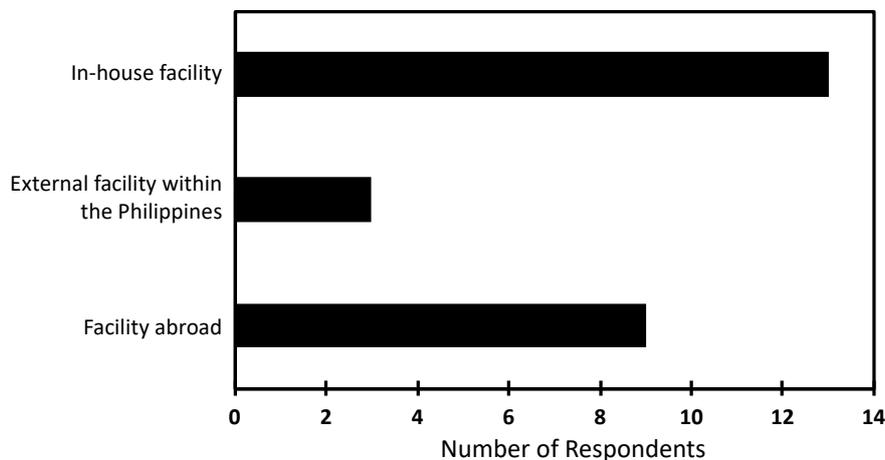

Figure 6: Number of respondents that perform calculations using in-house facility, and external computational facilities within the Philippines and abroad.

In the field of computational materials science, one crucial requirement for the conduct of research is the availability of computational facilities that can be used for calculations. Figure 6 shows the number of respondents who perform their calculations using their own in-house facility, and external facilities within the Philippines and abroad. It can be noted that most respondents have their own in-house facility while very few respondents perform their calculations to external computational facilities within the Philippines. Based on the survey, the only external computational facility that the respondents have used in the last five years is housed at the DOST – Advanced Science and Technology Institute (DOST-ASTI). It can also be seen from Fig. 6 that more than half of the respondents have access to external computational facilities abroad. These external facilities can be found in countries such as Japan, South Korea, Taiwan, and USA. The survey shows that five out of the earlier mentioned six respondents who have maintained a linkage with their foreign alma mater can access the computational facilities of such foreign institutions. This further signifies the existence of a follow-up linkage and collaboration among the respondents who have received their highest educational degrees abroad.

To establish a general picture of the specific calculations being performed by the respondents, the survey also explored the modeling and simulation methods and implementations that the respondents have been conducting. It was found that fifteen out of sixteen respondents use DFT as a modeling approach to materials simulation, indicating the popularity of this approach among the respondents. This agrees with the earlier mentioned wide usage of this approach in materials modeling as evidenced by the increase in the DFT-based publications in the past years. MD and kMC methods were identified to be used by 56.3% and 25% of the respondents, respectively. Among the respondents that utilize DFT, 67% use the Quantum Espresso software package, making it the most popular computational software among the respondents. Such software is based on plane wave basis sets and pseudopotentials, and is distributed for free under the GNU Public License (Giannozzi et al., 2009). The commercially licensed VASP (Vienna Ab-initio Simulation Package) (Kresse and Furthmuller, 1996) is used by 47% of the respondents that utilize DFT. The lower number of respondents who use VASP compared to Quantum Espresso can be attributed to the cost of licensing fee required for VASP. For computational chemistry software

packages, GAMESS (General Atomic and Molecular Electronic Structure System) (Barca et al., 2020) and Gaussian (Frisch et al., 2016) are used by 20% and 13% of the respondents that utilize DFT, respectively. As similarly noted for periodic calculations softwares, more respondents are using GAMESS because it is freely available for researchers. The most popular molecular dynamics software package is GROMACS (GROningen Machine for Chemical Simulations), which is used by 32% of the total respondents. It is also a free software and is available under the GNU Lesser General Public License (Abraham et al., 2015). These results have generally shown that the respondents have been using the freely available softwares more than the commercially available ones.
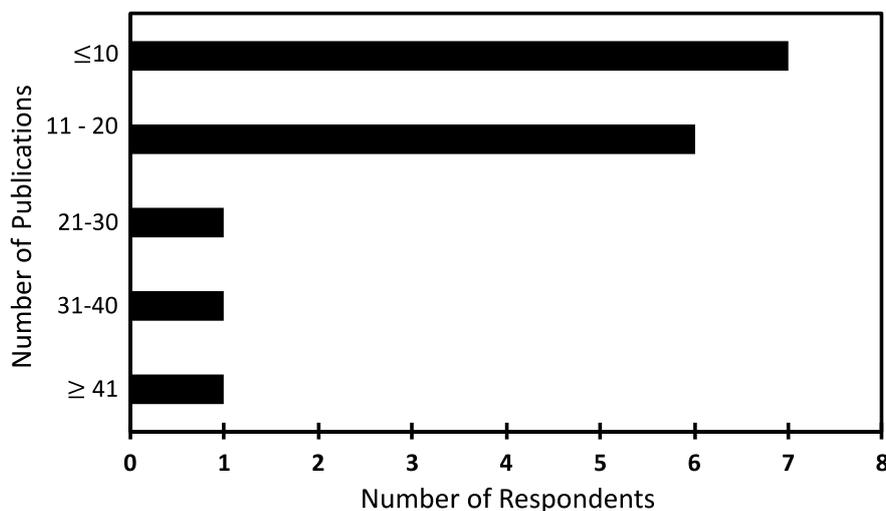

Figure 7: The range of the number of publications related to materials modeling and simulation reported by the respondents.

With regard to research outputs, one indicator of research productivity is the number of publications that the research groups have produced, as well as the presentation of their results in scientific conferences and conventions. Figure 7 shows the range of the number of papers published by the respondents as they have reported in the survey. It can be seen that most of the respondents have published 20 or less papers. The most commonly mentioned journals where the respondents have published their works are foreign-based journals by publishers and organizations such as Elsevier, Institute of Physics, American Institute of Physics, Physical Society of Japan, American Physical Society, American Chemical Society, and Royal Society of Chemistry. Some Philippine-based journals were also mentioned such as Science Diliman, The Manila Journal of Science, Philippine Science Letters, and Proceedings of the Samahang Pisika ng Pilipinas. With regard to presentations in conferences, twelve out of the sixteen respondents stated to have presented their research abroad in the last five years. For local conferences, nine out of sixteen respondents declared that in the last five years, they have presented their research at the annual national convention of Samahang Pisika ng Pilipinas (SPP). On the other hand, only three out of sixteen respondents have presented their research at the annual Philippine Chemistry Congress. This indicates that these experts are more likely to present their research in the physics community than in the chemistry group. Such observation is expected, considering that there are more respondents from the Department of Physics than from the Department of Chemistry.

PROBLEM AREAS AND RECOMMENDATIONS

The general picture that emerges from the survey is that the computational materials modeling community in the Philippines comprises only a small part of the overall scientific community in the country. There is only a handful of identified experts in this field and most of them are concentrated in the NCR. To identify the problems areas in this field faced by researchers in the Philippines, the respondents were asked about the difficulties and challenges they face in conducting research in the field of materials modeling in the Philippines. The answers of the respondents can be categorized into five areas as follows:

1) Infrastructure: The most frequently mentioned challenge among the respondents is related to computational infrastructure. Here, 69% of the respondents stated their challenges on having to establish their in-house computational facility rather than having a centralized national facility, difficulties in acquiring machines due to the procurement law, inadequacy of in-house facility for large-scale simulation, and unstable/unreliable internet and electricity. Among these challenges related to computational infrastructure, the difficulty of acquiring machines due to the prevailing procurement law has emerged to be a major issue identified by 19% of the respondents. Considering that materials modeling and simulation require high computational cost, the identified inadequacy of existing computational facilities by the respondents will significantly hinder the seamless conduct of their research.

2) Funding. 31% of the respondents mentioned challenges related to funding. One respondent stated that materials simulation has a low priority in funding deliberations because the funding agencies in the Philippines are apparently looking for immediate applications or economic gains (such as marketable products) out of pure science research. This puts the field of materials modeling at a disadvantage compared to other fields where prototypes and marketable products are relatively easier to develop. Furthermore, one respondent mentioned the lack of research grants that are allocated purely for computational modeling and simulation. It is noted from the survey that only 50% of the respondents have received research grants from the national government through agencies such as the DOST and CHED. It appears from the survey that those who availed grants from these government agencies have either partnered with experimental groups or provided provisions for future collaborations with experimentalists in the succeeding stages of their research.

3) Students: As earlier mentioned, most respondents have mentored only five or less students across academic levels. Such lack of significant number of students was also identified by the survey to be a problem area. Respondents have mentioned that there is only a small number of students who are interested to specialize in this field. Furthermore, one respondent stressed the difficulty of training graduate students because of insufficient undergraduate academic preparation. Because students comprise a significant workforce in a research group, a minimal number of students in this field will affect the overall research outputs of the group.

4) Administrative and teaching assignments: Respondents have also mentioned their work related to administrative and teaching assignments as a challenge or hindrance to conducting research. It is noted that several respondents have held or currently holding administrative positions such as dean, unit director, or department head. Moreover, all of the respondents have teaching loads that take up a significant amount of their time. Considering that conducting research and mentoring students require a substantial amount of time, an administrative position or a heavy teaching load will significantly interfere with research.

5) Collaboration with industry: It is noted that none of the respondents have declared having a collaboration with industry. The identification of this problem area in the survey indicates the very

weak linkage between computational materials science research conducted in the academe and the actual development and utilization of materials in the industry.
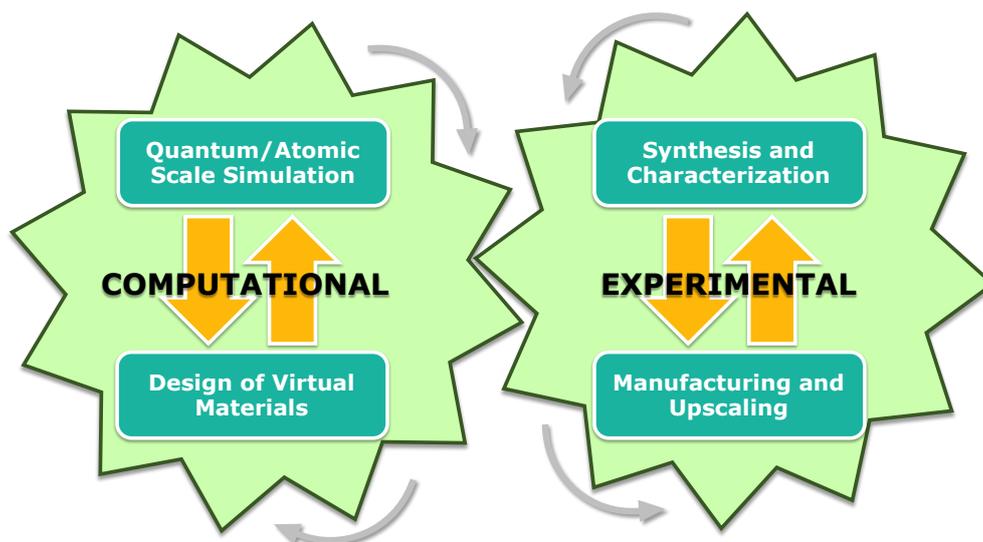

Figure 8: A framework for a complementary computational-experimental approach to materials science research.

Considering these identified problem areas from the survey, the following recommendations are proposed:

1) Secure the role of computational materials science in the National R&D Agenda: In the Harmonized National Research and Development Agenda (HNRDA) of the DOST for 2017-2022 and its corresponding Roadmaps, provisions for the use of computational materials modeling and simulation were included in the sector of Industry, Energy and Emerging Technology. Among the research priority areas in this sector, materials modeling and simulation can be extensively used in the area of renewable energy and energy storage solutions. Specific priorities in this area include the study of alternative energy sources to fossil fuels, adaptation and adoption of renewable energy systems, and development of functional materials for energy applications. In order to secure the role of computational methods in this priority area and other related fields, it is imperative to espouse a wholistic approach to materials science, where the complementary computational and experimental methods will be utilized. As shown in a proposed framework presented in Fig. 8, the computational and experimental "gears" should propel each other to find novel solutions to materials design that take advantage of the complementary results from these two overarching methods. The computational component of the research can provide an electronic and atomic scale understanding of the mechanisms that govern the physical properties of materials, thereby serving as a foundation for the computational design of virtual materials. The experimental component will take the inputs from computational results to gain insights into the synthesis and fabrication of materials, that will aid in the development of prototypes, and ultimately in the manufacturing and upscaling of products. In the past years, such integrated computational and experimental approach to materials science has yielded a significant number of high-quality publications, patents, and marketable products, and has strengthened the collaborations between computational scientists and experimentalists (Jain et al., 2016).

2) Enhance the high-performance computing facility at the DOST-ASTI for materials science: The DOST-ASTI is a government agency that houses a high-performance computing facility that can be used by researchers in the Philippines. Based on the survey, it appears that only three out of sixteen respondents submit their calculations at such computational facility in the DOST-ASTI, with some respondents even mentioning the lack of a national computational facility in the

Philippines. At present, the COARE (Computing and Archiving Research Environment) computational facility of the DOST-ASTI has mainly catered to the computing requirements of numerical weather prediction, climate modeling, bioinformatics, as well as data mining and analytics (COARE, 2020). Strengthening the access to the computational facility of the DOST-ASTI for materials science will provide better opportunity for researchers conducting materials modeling and simulation to conduct large scale calculations that would otherwise be very difficult to perform using only their in-house facilities. It is recommended for the DOST-ASTI to have a tenured expert manpower in computational materials science who can serve as a national focal point among computational materials scientists in the Philippines and to institutionalize a comprehensive R&D project solely in this field. Moreover, it is highly recommended for the national government to allocate sufficient budget for the upgrade of the current computing power of the COARE facility. Established in 2014, such facility currently has 864 cores, with CPU and GPU computing capacities of 30 teraflops and 72 teraflops, respectively (Delos Reyes, 2018). By comparison, one of the most powerful supercomputers in the world that is housed in the Oak Ridge National Laboratory has an impressive 148.6 petaflops computing power with 2.41 million cores, while the supercomputer Fugaku developed by Fujitsu and RIKEN in Japan has a theoretical peak speed of roughly 530 petaflops (TOP500.org, 2020).

3) Amend the procurement law in support of research: Under the 2016 Implementing Rules and Regulations of Republic Act 9184 or the Government Procurement Reform Act, necessary rules and regulations were prescribed for the modernization, standardization, and regulation of the procurement activities of the Philippine government (RA 9184, 2016). As earlier shown, since most research activities are publicly funded, the acquisition of necessary equipment for research needs to follow the procurement law. However, the stringent procurement procedures and amount of time it takes to procure an equipment have hindered the optimal performance of many research groups. Such problem in the procurement law is also observed in other fields of science and technology, as well as in other government institutions (Tumampos, 2019; Navarro and Tanghal, 2017). Among other things, the revision of the procurement law should provide simplified requirements and streamlined procedures that take into consideration a special provision for acquisition of research-related equipment, fast-tracked bidding process and failed bidding measures, and shortened procedures for foreign companies that do not have local partner agencies.

4) Dedicated funding for computational science research: While collaborations with experimentalists are expected to yield significant research outputs, there is a need to have grants dedicated for computational science research. This will address the earlier noted result from the survey that specifies the apparent bias against computational studies that do not yield an immediate marketable product and economic impact. Such research funding will provide researchers the liberty to explore unanswered questions in materials science with no regard to their immediate commercial viability. History has proven that many "curiosity-driven" pure science research in the past have only found applications after many years from its conception. One familiar example in the field of materials modeling is the case of DFT calculations, whose formalism was laid in the 1960s but only became a common method for materials modeling upon the development of powerful computers in the 1990s (Hohenberg and Kohn, 1964). Considering that the National Research Council of the Philippines (NRCP) is mandated by Philippine Legislature Act No. 4120 to support research studies that are primarily geared towards developing scientific knowledge of any subject, which may or may not have immediate practical applications (NRCP, 2014), the budget of the NRCP should be increased to be able to grant more research proposals that are purely computational in nature.

5) Establish a junior research group leader fellowship: In many universities and research institutions, senior researchers and faculty members are given administrative positions that interfere with their actual research activities, as earlier mentioned to be a problem area experienced

by the respondents. Because of this, it is recommended to provide the younger generation of researchers the opportunity to lead an independent junior research group dedicated solely to conducting their own research programs. Junior group leaders are competent researchers who have already gained substantial research experience (such as a postdoctoral research) after completing their doctorate. Through fellowship grants that can be jointly funded by the national government and local institutions, junior research leaders will have the opportunity to manage a research group, mentor students, independently realize a research project, and assume budget responsibility. Moreover, because of the small age gap between student mentees and junior group leaders, the fellowship may provide a more conducive environment for effective communication and unrestrained deliberation between the group leader and its members.

6) Establish an organized materials modeling community and networking: Among other things, an organization for materials modeling is important for two reasons. First, this can serve as a venue for sharing methods, best practices, public engagements, and trainings among the different subgroups of a wider materials modeling community (such as between scientists and engineers/technologists, physicists and chemists, submicroscopic and continuum scale simulations, and so on). It can also facilitate communication and cooperation links between industry, research, and academia. Second, an organization in this field will be instrumental to the development of a research roadmap for materials modeling and simulation. Such roadmap does not currently exist for the Philippines.

7) Strengthen computational materials science research in the regions: Considering that most of the identified experts in computational materials science are concentrated in the NCR, this field of research should be strengthened in the regional areas of the country. This will decentralize the expertise in the field, which will provide an opportunity for graduate students and researchers in the regional areas of the county to be mentored and trained in this field. One recommendation is to establish a regional niche for computational materials science in each of the Visayas and Mindanao regions. Recently, a DOST-funded high-performance computational science laboratory was inaugurated at the University of San Carlos in Cebu City, which was dubbed as the first computational science laboratory in the Visayas (Newsbyte.PH, 2020; Francisco, 2020). Such facility should be groomed to serve as a regional center for computational materials science by providing sufficient funding, scholarship grants for students, and training of expert manpower.

While this paper was focused on quantum and atomic scale materials modeling and simulation, similar policy recommendations may be adopted in other fields of science and technology in the country, which may also share analogous problem areas. It is hoped that this work will stimulate further interest in advancing the field of computational materials science in the Philippines.

CONCLUSON

In this paper, the current status and the overall research landscape in the field of quantum and atomic scale computational materials modeling and simulation in the Philippines is explore by administering an online survey form to sixteen identified expert-respondents. It was found that the computational materials modeling community in the Philippines comprises only a small part of the overall scientific community in the Philippines. Based on the survey, the identified problem areas in this field include the inadequate computational infrastructure, issues on funding, problems with students, administrative and teaching assignments, and lack of collaborations. Considering these results, policy recommendations aimed at advancing this field in the country were formulated. These recommendations include the adoption of an integrated computational and experimental approach to achieving the national research and development agenda in science and technology, enhancement of the national computing facility to include computational materials science as one of the priority areas for computation, amendment of the national procurement law

to ease doing research in the country, generate funding dedicated to computational science, establishment of a junior research fellowship and an organized materials modeling community, and development of regional niches for computational materials science that have sufficient funding, scholarship grants for students, and expert manpower.

CONFLICT OF INTEREST

The author declares no conflict of interest.

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