FROM MOLECULAR- TO PLANT-SCALE COMPUTATIONAL-ENGINEERING DESIGN: APPLIED TRAINING SPANNING SCALES

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INTRODUCTION

In his outlook on life, the 3rd-century BC Chinese Confucian philosopher and teacher, Xun Kuang, known more contemporaneously as "Master Xun" (or "Xunzi"), was known to have said, insightfully and sagely, in his teachings and philosophy:

不闻不若闻之，闻之不若见之，见之不若知之，
知之不若行之；学至于行之而止矣

Roughly translated, this means, "Not hearing is not as good as hearing, while hearing is not as good as seeing, and seeing is not as good as knowing, while knowing is not as good as acting; true learning continues until it is put into action."

Well over two thousand years later, remembering and galvanized over the centuries by those words by both formal teaching and more vocational training, under- and post-graduate education can be ameliorated by more active learning,[1] e.g., "flipping" the teaching engagement.[2] In general, comparisons between more active and passive learning styles are important, bearing in mind that active learning has been demonstrated statistically to yield greater levels of more meaningful subject comprehension, in tandem with general critical awareness.[3] This is particularly true in the area of training and education in engineering,[4] for which more passive and vicarious teaching-and-learning experiences are becoming increasingly outmoded and documented as being less effective.[5] A powerful exemplar of this active-learning approach "in action" is hinged on the application of Problem-/Project-Based Learning (PBL) methods. This is in contrast to more established lecture-and-tutorial approaches (with the occasional laboratory practical session) – developing more engaged engagement with key learning outcomes in engineering courses.[6]

Generally, apropos engineering-education training efforts in and of themselves, including the question of how best to handle and approach shorter courses suitable for working professionals, a number of desiderata have been highlighted vis-à-vis improved results.[7] This includes, amongst other points, deeper interest in technical science/engineering data analysis for working engineers and empowering industry in terms of greater technical competence and overall confidence in data-intensive handling and numerical-/computer-aided engineering design. In particular, for scientific and engineering outreach programs,[8] this affords developing general engineering skills, e.g., communication and teamwork. In this case, it is clear that PBL constitutes an effective tool to ameliorate professional training.[5]

There have been rather commendable advances in recent years of more active learning approaches – often in the guise of PBL as an expression of this method. Here, however, embedding PBL and active learning into computational-engineering training, whether to under- or post-graduate students at third level (equivalent to graduate-level students in the US) or else to working engineering professionals in shorter, more focused courses, is less developed. Despite this, there has been progress recently in this arena.[5] Expanding this general theme, assessing what kind of lessons can usefully

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shape third-level (graduate-level) training, e.g., influencing curricula, programs and active-learning modalities in data science and numerical approaches (especially at different scales), is relatively less explored.

Considering this comparative gap in the literature, the data-intensive training agenda constitutes an interesting approach to ascertain how active learning, careers stimulus, and industry-engagement initiatives for working engineering professionals can inform the university sector, improving future engineering-teaching standards.

The present study centers around active learning in "buzz" groups (i.e., groups of 2-3 students working actively and intensely in-class on a particular sub-step of a problem) for engineering postgraduates and working professionals. This is done to expose concepts in gas- and materials-engineering using PBL approaches, observing their peer interactions to develop university-level lessons on active learning in data-intensive areas and subjects. In addition, industrial-outreach efforts have led to conclusions vis-à-vis motivations towards data-intensive gas- and materials-engineering education and training, which support the redesign of gas- and materials-engineering curricula for more active learning. In a very strong sense, this twin pillars of activity overlap in scope and intent with the philosophy of Kolb's experiential-learning cycle,[9] in that both seek to have at their heart a more active-learning philosophy. Bearing both goals in mind, these twin initiatives offer lessons and conclusions for improving engineering education and training centered around data science.

PROBLEM-BASED LEARNING

Student Engagement

In order to advance the strand of PBL and experiential approaches in data-driven learning in gas engineering, we encouraged students to form rival "buzz groups" to work on a PBL projects in the general area of gas engineering.

More specifically, clathrate hydrates are crystals not dissimilar to ice in appearance, wherein guest molecules are entrapped.[10] These guest molecules can differ widely, although methane clathrates are most common (Figure 1). They are in nature mostly in permafrost and seafloor milieux. Recent success at direct hydrate production with a depressurization method at the Nankai Trough is encouraging. That being said, since methane has roughly a 20-times-larger capacity to keep atmospheric thermal energy compared to CO_2, relatively minor leakage of CH_4 from natural hydrates is a huge problem. Hydrates also tend to block gas pipelines, owing to the presence of water vapor therein and the thermodynamic stability of hydrates at these temperatures and pressures - most especially at temperatures above 0 degrees Celsius. Keeping gas flowing through pipelines without hydrate blockage is a key priority for the gas industry – "flow assurance".

Having introduced the concept of gas hydrates in gas engineering, in the computational PBL assignment project (featuring occasional in-class 'buzz' groups), the post-graduate students were motivated in their data-modelling projects by scale-spanning activities. In Figure 2, we provide an example of clathrate hydrates as a problem in gas-pipeline flow assurance, in that their formation may cause pipe blockages. One of the core themes of these modelling PBL projects is the scale-spanning nature of hydrates in gas-engineering operational troubleshooting and design challenges.

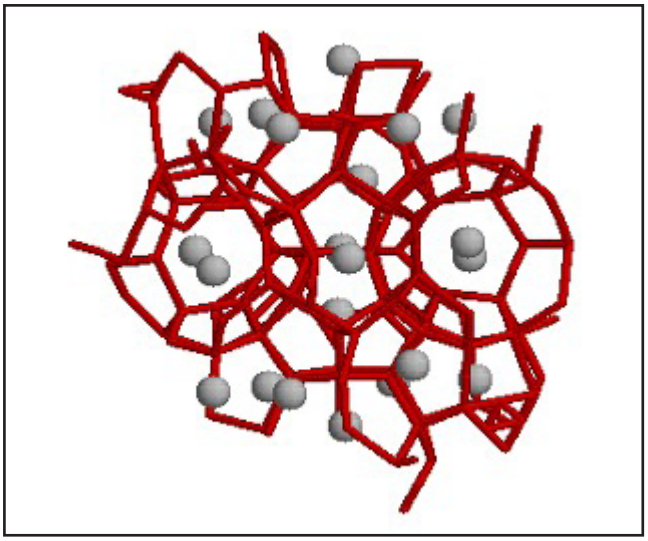

Figure 1. *Hydrate nano-sized cluster, showing pentagonal and hexagonal faces surrounding methane molecules in cages.*

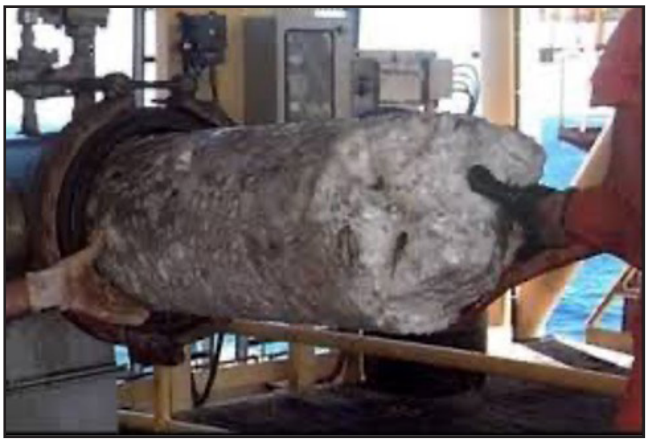

Figure 2. *Clathrate-hydrate plug in a gas pipeline. Often, silica particles in the gas stream serve as heterogeneous-nucleation sites [9]*

Nature of the Data-Intensive Projects

As the adoption of computer-aided modelling and process simulation have become more generally widespread, they have also become yet more embedded in industrial engineering design. This includes the exploration of how multi-scale molecular-, fluid- and field-dynamics simulation fits into the overall corpus of education, training and industrial practice – and how this has been shifting in recent years.[11] In particular the positive role of the AIChE Computational Molecular Science and Engineering Forum is to be acknowledged here. In any event, the molecular-simulation/modelling PBL projects were to harness the power of integrated process simulation across scales – from the molecular to pipelines.

The students, in the spirit of PBL[5] and Kolb's general experiential-learning philosophy,[9] had a certain level of freedom in being able to define a project and its goals. However, the general theme and route were adopted of being able to use molecular simulation as a pragmatic and predictive-design tool in prototyping and trialing flow-assurance strategies in pipelines. In the leading contender for most insightful scale-spanning project, the small group of postgraduate students took a three-pronged approach:

1. identifying by molecular modelling the spinodal-decomposition compositions and conditions of methane in water (with silica "dirt" particles entrained in the wet-gas flow often serving as sites for heterogeneous nucleation of clathrate-hydrate nano-crystallites atop). This was done by means of a DL-POLY-based [13] molecular simulation of methane-water-hydrate interfaces with a simulation box capable of accommodating up to 12-15 unit cells of sI methane hydrate [12] – see Figure 3.
2. prediction by computationally-intensive molecular simulation of the hydrate-nucleation free-energy barrier so as to characterize the thermodynamics and energetics of hydrate nucleation and formation in gas pipelines. This was accomplished by the well-tempered metadynamics [14] approach with DL-POLY [13] to map out the free-energy surface with the water-methane potential models of ref. 12 – cf. the conceptual schematic in Figure 4 for further details, including system size.
3. relating computationally to flow-assurance in pipelines, in terms of blockage/plugging probability, and informing the design of plugging-mitigation/avoidance strategies. This was carried out by modifications to the multiscale approach advocated in ref. 11, whereby the multiscale-modelling paradigm had its boundary-value treatment extended to take DL-POLY simulation [13] inputs.

Assessment of Value

In terms of formative assessment, a questionnaire afterwards found that about 75% of students expressed enjoyment and satisfaction with the PBL-based computer-modelling exercise. However, this statistical data was not taken in the case of a remote-

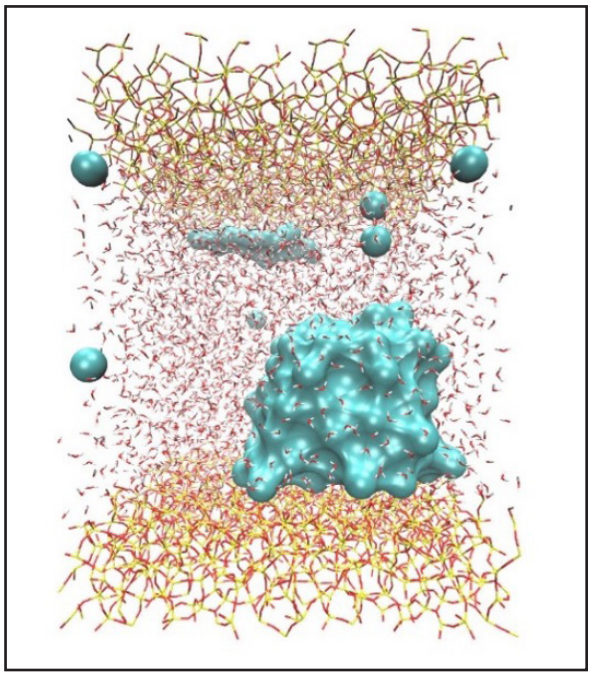

Figure 3. *Molecular-graphics visualization of the onset of spinodal decomposition of a methane nano-bubble[12] in contact with a silica surface of the type encountered under industrially relevant heterogeneous-nucleation conditions.[10] This computational analysis allows the onset of hydrate-nucleation conditions to be assessed in greater detail, such that nano-crystallites of the type shown in Figure 1 (near a critical size, cf. Figure 4) can be predicted and modelled by molecular-simulation means. These simulations were carried out using water-methane force-fields [12] in the DL-POLY [13] software, and using the well-tempered metadynamics using the hydrate-crystallite diameter as the essential order parameter.[15] Thus, a piece of amorphous silica with dimension 25x25x25 Å previously relaxed at 1 atmosphere and 298 K was replicated 4 times, two and two along the axes x and y. The so obtained system was equilibrated for 1 nanosecond at 260 K and 500 atm. The intra- and inter- molecular interactions were modeled by the CHARMM potential, specifically developed for silica bulk [16]. Finally, the so obtained simulation box of approximately 50x50x25 Å was cut following the plane x-y at a z value equal 12.5 Å, and along the cutting surface a volume corresponding to a orthogonal box of dimension 50x50x42 Å was added. A simulation box of approximately 50x50x67 Å was thus obtained, comprising along the z axis of 25 Å of silica bulk and 42 Å of vacuum, which was later filled up with a mixed H_2O/CH_4 fluid. Note that the surface cut was performed along the oxygen bridge connecting two silicon atoms of the silica bulk, which was found to be the lowest-energy configuration for this surface construction.*

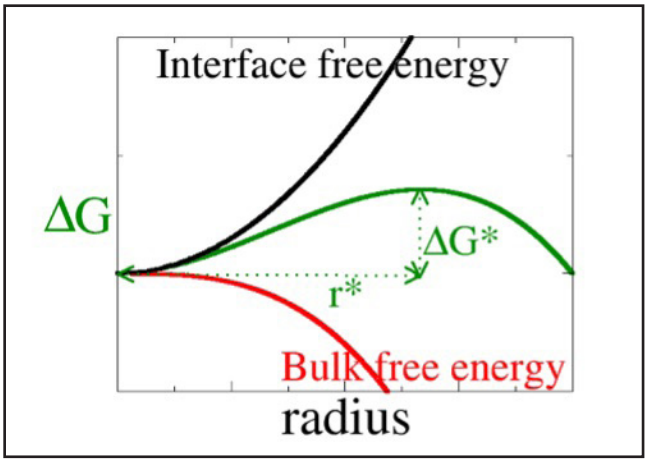

***Figure 4**. Conceptual schematic illustrating the overall qualitative trend in the variation of the nucleation free energy with crystallite radius for the development of a critical-sized nano-crystallite similar to that depicted in Figure 1. Once the interfacial and bulk free-energy terms are subtracted to take the difference for the free-energy work of forming a crystallite, they combine to be maximal at the nucleation free-energy barrier, ΔG*.[10] Knowledge of the nucleation free-energy barrier helps to predict macroscopic hydrate-formation rates.[10]*

conduct example (which occurred in 2020-2021, owing to the COVID-19 pandemic curtailing ready access to colleges, schools, and universities, and, indeed, the physical closure of many such institutes in Ireland and the use of online remote training-education). Still, in the case of that remote conduct of the data-intensive project, qualitative feedback from the students was positive and engaging. The relative freedom to develop the hypotheses and methodology, and use numerical modelling software to address challenges in multi-scale ways, were seen by students as being the most interesting aspects.

PROFESSIONAL DEVELOPMENT AND DATA-MODELLING PBL

Context

Developing the theme of data science further has become a goal in the context of taught postgraduate programs in the School of Chemical and Bioprocess Engineering at University College Dublin (UCD). This is in keeping with one of UCD's guiding themes (2019-24) of digitalization in its overall teaching and research missions. Based on positive recent experiences in chemical engineering education of PBL,[17] together with this general background of increasing engagement with digital and computer-aided design approaches, the use and deployment of high-level scripting and graphical computing have become mainstream tools for process engineers[18] to harness the power of integrated complex process-plant simulators in a multi-scale manner. In a similar spirit to the previous section, embracing scales in digital-based process modelling, from the "molecular to the macro" has become a guiding principle or theme in program and curriculum design. In this sense, and from this perspective, this section shall describe the conceptual development at UCD Chemical Engineering of both an emergent 90-credit (ECTS) taught-Masters program and a 20-credit professionally-oriented Certificate. (An Irish credit, ECTS, is double the US-based credit.) This is to cater for both on-campus and professional, practicing engineers wishing to develop skills in data-driven modelling at various scales.

Rationale

One of the central themes of contemporary chemical engineering, and currently one of the pillars of the UCD School of Chemical and Bioprocess Engineering's strategic plan, is the fabrication and design of novel functional materials and molecular devices for applications in a broad range of chemical and electronic systems. The latter include chemical and optical sensors, medical devices, drug-delivery systems, pharmaceuticals, nano-particulates and powders, selective nano-membranes, photovoltaics and catalysts. This is to cater for a very broad variety of chemical and photochemical transformations of materials and energy. Although there are many programs internationally that are focused on the delivery of engineering training in the manufacture and development of bulk materials, it is evident that few programs address interfacial systems and the unique tailoring of such systems in a directed way. In Ireland, at this time, the major established industries with which the school interacts include (bio-)pharmaceuticals, medical devices and IT. However, in addition to multinational corporations within these areas, in the last decade there has been the welcome development of a growing number of small-to-medium sized enterprises that are providing opportunities for graduate employment. This includes chemical synthesis, heterogeneous catalyst design, photonic and photovoltaic (PV) devices and thin-solid-film processing. With the strong emphasis by the Irish government on foreign direct investment, as well as its recent prioritization of directives within processing technologies, novel materials and manufacturing competitiveness, it is anticipated that the need for training of engineering graduates will grow rapidly in the coming decades. This will include opportunities in research within the field of functional materials in interfacial systems. This is especially true considering device development and manufacturing considerations, and, clearly, scale-spanning data science and simulation will play an important part of this. In this, exploiting simulation as a predictive materials-design tool as applied to interfacial systems at multiple levels will be important.

From educational, pedagogical and ultimate-applications perspectives, the topic of the emergent Interfacial Engineer-

ing of Advanced Materials (IEAM) impacts on the activities of a number of major groups in the School and across UCD. From this perspective, we believe that the modules offered within the MEngSc program will be of significant value to other taught programs (both in Ireland and internationally). The facilities available to the school, both experimentally and computationally, to achieve a high educational standard in the program's field of training are strong. In particular, the school is equipped with a comprehensive range of world-class materials-processing and characterization facilities, which will be central to the students' educational experience.

This developing MEngSc program (IEAM) is relatively unique on the international scene. The important distinction between it and other materials-based taught-Masters programs is that it addresses the need for a program focused on the design, tailoring and characterisation of materials in and at interfacial systems spanning fundamental electronic/atomistic principles to macroscale engineering manufacturing processes. In this regard, this program complements the ME in Materials Science and Engineering within the UCD School of Mechanical and Materials Engineering. That primarily addresses technologies associated with bulk materials (e.g., thermodynamics, kinetics and continuum/constitutive properties and manufacture), along with most other materials-based taught-Masters degrees internationally. However, this IEAM MEngSc considers solid/fluid interfacial systems, surface-modification issues and interfacial characterization, together with the response to external stimuli of direct relevance to Chemical and Surface Engineering. Indeed, this is ripe for molecular simulation and other physics-based modelling of interfacial phenomena.

The applications of Interfacial-Systems Engineering are clear in a broad spectrum of industries in Ireland, and internationally, today. To that end, opportunities for employment exist in many companies and industries that contribute significantly to the Irish and international economy, including in the rapidly-developing field of industrialization of nano-bubbles in interfacial systems,[12] with strategic partner Aqua-B. In light of the above, this IEAM program is poised to be of strategic and critical importance to the school and college in the future, while promoting training and education in a nascent field of interfacial engineering with very strong potential for a data-science-driven "molecular-engineering" focus.

The Professional-Engineering Audience

Given the highly specialized technical audience of this MEngSc, which is so pivotal to the training of an advanced workforce in many industrial sectors in Ireland and internationally, another core impetus and motivation lies in catering for those in industry wishing to take some important data-/modelling-friendly thematic courses in advanced materials for interfacial systems. Here, the emphasis is on developing a reduced core, 'skeletal', offering of a Postgraduate Professional Certificate, allowing for potential further scope upon which this "scaffold" could be later built. This would be particularly so if there is an appetite by the professional student to progress, in and over time, to an MEngSc in IEAM. In spirit and in essence, this pays close, pragmatic attention to 'upskilling' demands from industry, e.g., training-program developments and enhancements to cater to these needs. If anything, this trend has been amplified by the COVID-19 pandemic, where remote working and training has emphasized the need for sophisticated computational-engineering design tools, often with a molecular focus. To this end, a data- and modelling-centric, practitioner-oriented program for part-time learning (typically remote) is being developed.

In this context, key goals and drivers are:

- realizing an 'integrated' vision, spanning the molecular- to plant-design scale
- achieving progress in professional multiscale computational-engineering training through academic-industry cooperation, ranging from undergraduates to practicing engineering professionals
- tailoring shorter, professional courses by academia in scale-bridging simulations for industry by academia

Make-Up of the MEngSc and the 20-credit Postgraduate Certificate

The course structure of the emergent MEngSc of Advanced-Materials Engineering for Interfacial Systems is summarized in Figure 5, including a 30-credit summer research project.

The 20-credit data-centric/modelling-focused Professional Certificate under finalization is centered around: (i) Computational Methods for Atomistic Modelling, (ii) Advanced Experimental Design, (iii) Biological Interactions with Materials and (iv) Nanomaterials. In the case of the first two courses for this certificate, these are predicated on exclusively molecular- and continuum-scale modelling, spanning from atomistic- to plant-level phenomena with multiscale modelling.

Case-Study Examples of Data-Driven PBL Projects

An example of a recent PBL assignment project (with occasional in-class 'buzz-group' brainstorming) in such interfacial-systems materials engineering involved investigating zinc-oxide nano-particles for electrolytic hydrogen production. This involved a good deal of atomistic simulation of the electronic-band characteristics of ZnO, as detailed in Figure 6, as part of a multi-faceted campaign to characterize more and better-performing ZnO nanoparticles for H_2 production.

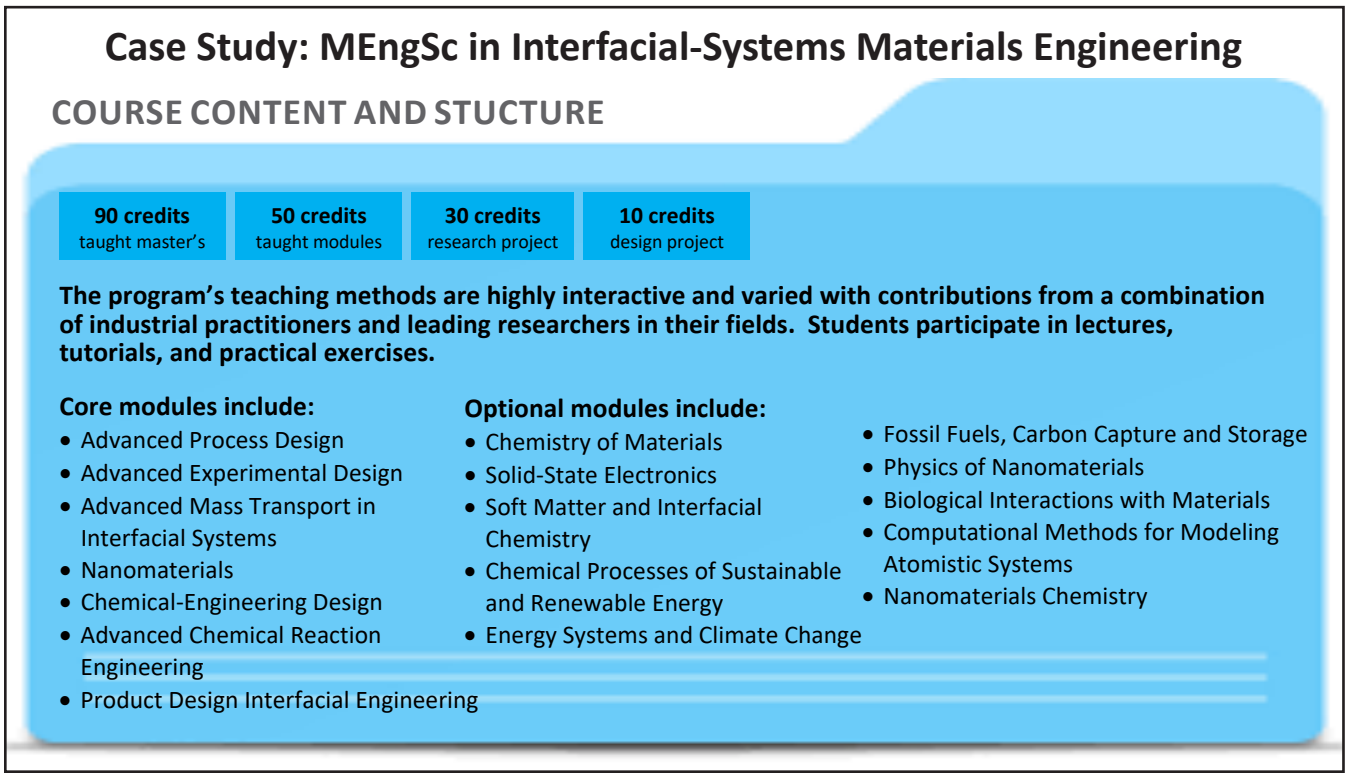

Figure 5. *A summary of the key course structure (90 credits ECTS) in the IEAM MEngSc over 12 months from early-September to early-September, which includes a 30-credit Summer research project from mid-May to late-August.*

This PBL project detailed in Figure 6 allowed students to improve the band-gap properties of the ZnO nanoparticles by varying the surface geometry and using experimental verification and measurement of the current-density under various bias potentials. This meant that molecular modelling for electronic 'personality' and characteristics of the material could be used as a prototypical materials-design strategy. This is of clear industrial relevance for interfacial engineering in industry. In surveys afterwards, the students' qualitative feedback was very positive, in that the freedom of the project, and in discovering and following computational approaches, allows them to understand much better the whole "molecular-engineering" project lifecycle, from concept to actual nano-scale engineered product.

A second industrially-relevant PBL assignment-project of key molecular-modelling interest is in crystal-structure prediction (Figure 7). Here, the postgraduate students can devise optimal strategies for developing "fit-for-purpose" force-fields that are most suitable for modelling these solid-state polymorphs.[19] This includes using machine-learning approaches with industrial partner BioSimulytics and then applying them to predict the most stable crystal polymorphs ranked against experimental data (with the understanding that experimental data are not guaranteed to have the lowest-lying polymorph energy). These PBL projects have led to impressive levels of learning among the cohort of students of the need to embrace the art and pragmatism of highly accurate force-fields. This is particularly so if one is to make meaningful progress in tackling the innately challenging problem of crystal-structure prediction.[19] In this, the students developed a multi-scale modelling suite of skills of high interfacial-systems interest in crystal engineering, of major interest to the pharmaceuticals industry.

For both of these demanding PBL projects, teams were assigned randomly, and there was close supervision by the instructor and industrial collaborators, with a good deal of explanation and tutoring in use of the codes. However, it was up the students to make the creative, high-level decisions of which particular approaches to use in making use of the library of codes.

It is informative and important to attempt to assess the value of these case-study examples, ideally from more than one perspective. PBL-survey questionnaires after the conclusion of these mini-projects concluded that about 80% of students found both of them to be very informative, and that this taught them new skills in computer modelling of materials. Qualitative feedback from project students was also positive. Indeed, some have gone on to seek employment opportunities and deeper postgraduate-research opportunities in these areas of materials modelling, given that the open-ended nature of these problems is more appealing in the sense of suggesting career-progression possibilities.

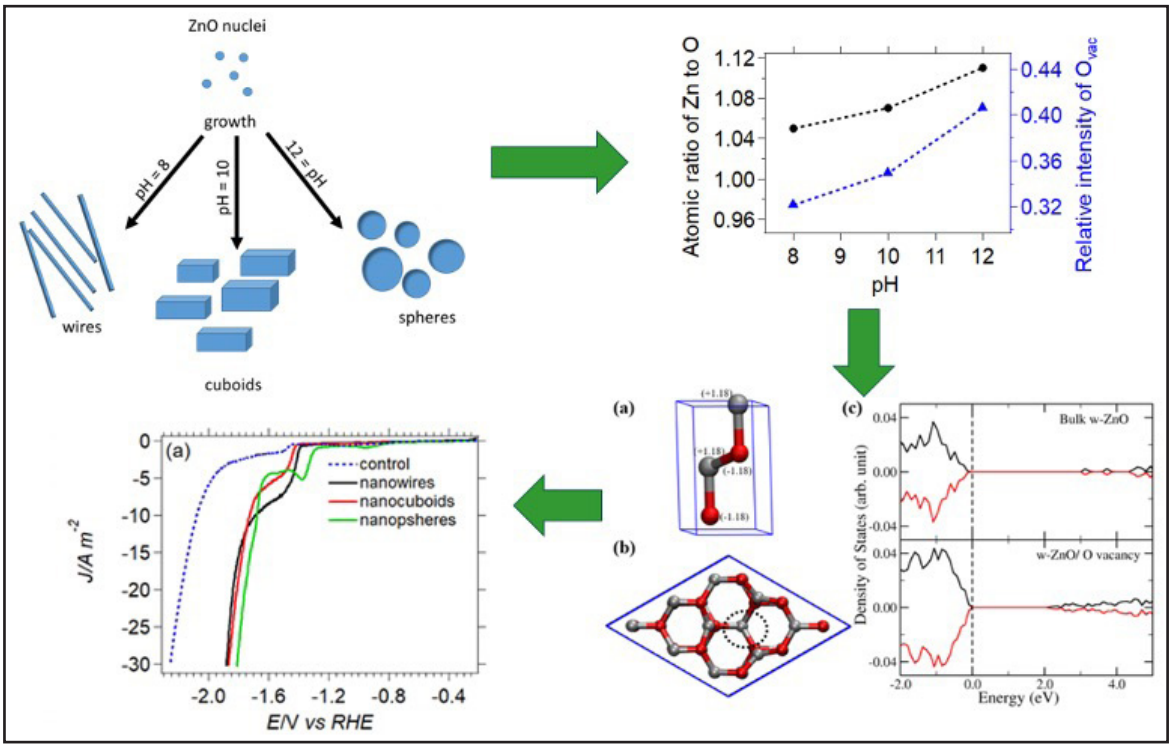

Figure 6. *Multi-faceted, multi-scale approach to PBL in assessing and improving H_2-production levels in ZnO nanoparticles. The molecular-modelling is emphasized in the bottom-right part of the figure, which relates the prediction of the electronic Density of States from the atomic structures shown, for both the case of bulk material, and as a function of vacancy concentration.*

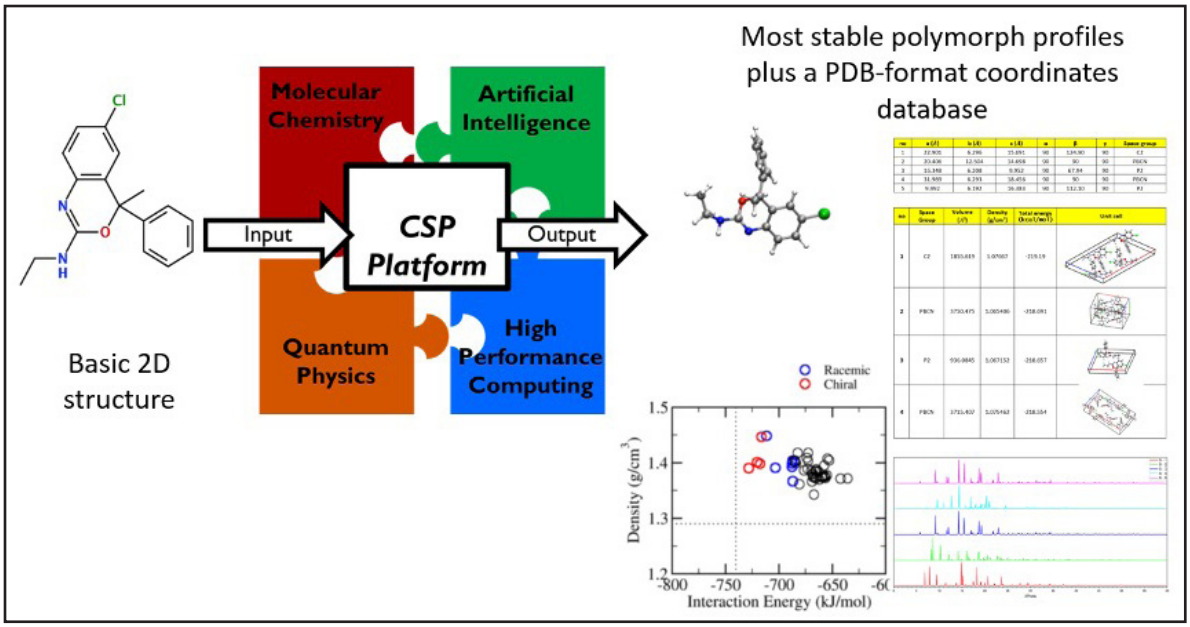

Figure 7. *Crystal-structure prediction using the basin-hopping method[19] in collaboration with industrial partner BioSimulytics. In PBL involving industrial collaboration, postgraduate students have a chance to develop tailor-made force-fields using machine-learning approaches. Then, they may apply these to predict the most stable crystalline polymorphs ranked against experimentally available data (noting that experimental data are not always guaranteed to be that of the energetically lowest polymorph).*

CONCLUDING REMARKS

In recent years, the power of computational design for molecular- and nano-scale engineering applications has become more clear, to the point of spawning yet more reliable molecular-design and prototyping tools. The present work has discussed some of these developments, albeit focussing on multi-scale simulation to emphasize industrially-relevant computational-design projects for practicing process engineers, with an eye towards "upskilling" demands from industry. This integrated simulation "vision," spanning the molecular- to plant-design scale, has been outlined in the case of program and curriculum design vis-à-vis the emergent MEngSc program in Interfacial Engineering using Advanced Materials, with the allied Postgraduate Certificate. Here, the role of multiscale simulation and computational involvement is pivotal, underpinning the central philosophy in the formation of students via PBL challenges into confident and technically competent practicing computational-engineering professionals.

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