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Emerging Materials, Computational Research Needs and Challenges for Alternative Energy Innovations

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Abstract

The demand for new energy technologies has greatly exceeded the capabilities of today's materials and chemical processes. To convert sunlight to fuel, efficiently store energy, or enable a new generation of energy production and utilization technologies requires the development of new materials and processes of unprecedented functionality and performance. New materials and processes are critical elements for progress in advanced energy systems and virtually all industrial technologies. Harvesting the potential of computational science and engineering for the accelerated discovery and development of disruptive technologies and an enchanted and integrated interplay of Computational Materials Science, Chemistry and Biology will definitely establish a new era of technology evolution. This paper shows advances and challenges in the field of computational materials science, smart materials and innovative approaches. It identifies what are some of the future trends and innovations that may make an impact on the world of energy.

Keywords:	Multidisciplinary computing; Emerging technology, Challenges, Material science

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1. Introduction

It is important not only to identify hardware and software technologies but also ideologies and legaslative that can affect significantlt how particular energy will rich a crucial mass in terms of impact of our lives. This paper is focused on importance of emerging computational science and impact of technologies being pursued for harvesting the renewable energy but also for developing disruptive technologies. The disruptions in technology development are enabled by a novel approaches of energy exploration and synthesizing multiple and multidisciplinary approaches in one intelligible and robust integrated system.

The objectives of this paper were to identify possible priorities and synergy trends (fundamental science, manipulation of materials through computational science and energy innovations) in the field of emerging energy technologies and to gather ideas on how to progress towards the successful development of materials with disruptive approaches. The paper provides a summary of information in references, identifies issues and problems that need to be addressed, and to some extent provides recommendations for new approaches to solving these problems. Also, the paper briefly touches the scientific contribution to solving the identified problems.

This technical paper is organised as follows. In the Chapter 2 the capability of predictability which is enabled through advanced computational science is discussed. The Chapter 3 deals with the challenges of technology complexity that were accelerated due to demands for more efficient harvesting the renewable and alternative energies. Particularly, the focus is given to controlling the material's micro- and nano-structures including the self-assembly. The Chapter 4 is devoted to challenges posed to PV cells. There we explored the theoretical, experimental and technological challenges

posed to organic polymeric and small molecules and inorganic nanostructure PV, as well as to the hybrid structures and the biomimetic materials. In the fourth chapter we tackle advantages of manufacturing the materials in microgravity environment. Conclusion is given in the last chapter.

2. Capability of predictability

The computational materials science tools, based in chemistry and physics, give us as follows: the qualitative frameworks for thinking about atomistic processes and mechanisms, the quantitative understanding of thermodynamic driving forces, and the prediction of the properties or molecular architectures for engineering design. Often, we want to know the structure of a few atoms in a material (e.g., defect or reactive sites), and quantum mechanics allows us to calculate these structures and associated electronic energies to high accuracy. However, we ultimately need to predict multi-scale properties that can be compared with experimental data, so we use statistical mechanics to perform temporal or spatial averages over a large number of simulations to obtain these macroscopic observables. We thus develop predictive insight that may be used to guide experimental design of new materials. The benefits of predictive capability in science and engineering are as follows. The scientific discovery process is not linear—it follows an often chaotic path of intuition, trial and error. Predictive capability accelerates discovery by guiding experiments in the most productive directions (as we saw in particle physics experiments and in nuclear industry), by reducing the number of options or configurations that need to be tried, by suggesting specific breakthrough opportunities for experimental verification, and by providing powerful tests for theories that improve fundamental understanding. In many cases, progress demands predictive capability due to the complexity that must be navigated. Capability of predictability of Computing Science is powerful tool in the transformation of technological innovation. Computing science not only predicts some material behaviour but can help to design novelty using novice approaches.

3. The challenge of complexity: The discovery of design with the mathematical modelling

The advanced materials are complex. Their development includes multiple chemical components, nanoscale architectures, and tailored electronic structures. The discovery is increasingly confronted with complexity, which cannot be explored only experimentally. Thus new materials and new chemistry have to be designed, using new synthesis, synergy and characterization tools, theory, and simulation and modeling to understand complex materials and chemical systems and predict the most promising research directions. Computational materials science and engineering has emerged as an interdisciplinary subfield spanning materials science and engineering, condensed matter physics, chemistry, mechanics and engineering in general. A number of computational methods and tools are developed, ranged from electric structure calculation based on density functional theory [1, 2], atomic molecular dynamics [3-4] and Monte Carlo techniques [5], phase-field methods [6-8] to continuum microscopic approaches. The Open Visualization Tool (OVITO), a new 3D visualization software designed for post-processing atomistic data obtained from molecular dynamics or Monte Carlo simulations is described in [9]. Transient current technique and appropriate simulation modeling is promising technique for studies of silicon detectors [10].

It is important to note that over last couple of decades the different trends in computational science in correlations to science of materials were developed. For instance, researches and approaches have been steadily moving from technique development and purely computational studies of materials towards discovering and designing new materials facilitated by computation, artificial intelligence such as neural networks and deep machine learning and data mining or by comparing and combination of computational prediction and experimental data/validation. The most resent trend emphasized the focus on design on discovery of new materials rather than on purely computational; technique improvement or purely theoretical understanding of materials structure and properties. One of Journal that support such initiative is Computational Materials [11].

The physical properties (mechanical, electrical) are often brought to the theoretical limits. What we now see is a new concept: discovery by design. Predictive modeling fosters design and testing. State-of the-art computational tools allow scientists to calculate from first principles the interactions that dominate microstructural behavior, while experimental tools can now provide time resolved measurements on real materials to validate these models. Integration of theory, simulation, and experiment accelerate materials discovery and innovation. Obviously, the keys to achieving these advances are verification, validation, and uncertainty quantification of the computer models. Thus, it is important to think and work from atoms to the bulk, and the divisions between disciplines (first principles theory to mechanical engineering) will start to dissolve. To achieve this goal one must be able to realistically simulate the physical phenomena over a vast range of time and length scales.

3.1. Controlling microstructure

Frankly speaking, simulation-based engineering is not a new concept. We now see only a new approach which employ an old concept on revolutionary new way, bringing chemistry, physics and biology to dissolve their boundaries into world of computational modelling.

The availability of structural materials that can operate at extreme values of temperature, stress and strain, pressure, radiation flux, and chemical reactivity is the principal limiting factor in the performance of many energy systems. Fossil power plants, nuclear plants, and transportation systems all operate at lower efficiencies due to the limitations of existing structural materials. Central to this challenge is predicting and controlling the microstructure—the complicated arrangement of crystalline grains, defects, interfaces, and impurities that make up the microscale structure. Microstructure is the key to understanding damage processes, preventing failure, and enhancing performance. State-of the-art computational tools allow scientists to calculate from first principles the interactions that dominate microstructural behaviour.

The microstructure of a material controls a wide range of important properties, including strength, fatigue, and high-temperature performance, corrosion, and radiation resistance. While there is substantial qualitative understanding of microstructural evolution, there are no predictive models that link materials processing to resultant microstructures.

The special emphasis is on the experimental verification of the theoretical predication and feedback to theory. For example, the broad range of imaging and microscopic tools such as optical microscope (Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Field Ion Microscope (FIM), Scanning Tunnelling Microscope (STM), Scanning Probe Microscope (SPM), Atomic Force Microscope (AFM), X-ray diffraction topography (XRT)), or spectroscopic (Energy-dispersive X-ray spectroscopy (EDX), Wavelength dispersive X-ray spectroscopy (WDX), Electron energy loss spectroscopy (EELS), Photoluminescence (PL), Photon correlation spectroscopy and dynamic light scattering (DLS), small-angle X-ray scattering, Ultra-visible light spectroscopy (UIV-vis, Small-angle neutron scattering (SANS) etc.) and many others provide information on material structure and functionality on macroscopic level and local levels. Systematic analyses and curation of these types of data will allow construction of libraries of structure-property relationship at atomic levels (similar concept used for decades in high energy physics analyses where each signal/track is assigned to different libraries and correlation between them through library manipulations allows scientists to perform physics analyses). This knowledge can then be incorporated in theoretical models by providing realistically observed defect configurations and providing refinement of theoretical model parameters.

Furthermore, there is a lack of understanding of the connections between microstructure and materials performance. The new generation of synchrotrons and neutron sources, and synthesis and characterization equipment, together with recent computational and algorithm advances, provides an opportunity for the first time to envision designing microstructures for specific purposes and bringing them to fruition in real materials [12].

3.1. Designing and engineering materials at the nanoscale: Understanding and controlling self-assembly

Structures whose constituents can assemble, disassemble, and reassemble autonomously or on command enable materials capable of self-repair, multi-tasking, and even shape-shifting—properties known throughout the biological world. By combining organic and inorganic matter into hybrid building blocks, hierarchically ordered nanostructures can be achieved through self-assembly.

Let us first define the meaning of self-assembly. According to [13] “Self-assembly is the process by which small components automatically assemble themselves into large, complex structure”. There are many examples as such: lipids self-assemble a cell’s membrane and bacteriophage virus proteins self-assemble a capsid that allows the virus to invade other bacteria. The study addressed the question “How could such a process be described as “algorithmic”?” It was clearly pointed out that since the meaning of algorithm is to automate a series of simple computational tasks, then, algorithmic self-assembly systems means that they automate a series of simple growth tasks, in which the object grown is simultaneously the machine controlling its own growth. So it becomes clear that the idea of “molecules that can perform computation” is transforming the way the engineer is self-assembling molecular systems. The systematic manipulation of information moves slowly to systematic manipulation of matter.

To emphasize the computational impact on controlling self-assembly we firstly summarize some of distinctive features of self-assembly materials [14]. The sself-assembling molecules adopt a structure at the thermodynamic minimum, finding the best combination of interactions between subunits but not forming

covalent bonds between them. Thus, in self-assembling structures, the scientist must predict this minimum, not merely place the atoms in the location desired.

Another characteristic common to nearly all self-assembled systems is their thermodynamic stability. For self-assembly to take place without intervention of external forces, the process must lead to a lower Gibbs free energy, thus self-assembled structures are thermodynamically more stable than the single, unassembled components.

A direct consequence is the general tendency of self-assembled structures to be relatively free of defects. An example is the formation of two-dimensional super-lattices composed of an orderly arrangement of micrometre-sized polymethylmethacrylate (PMMA) spheres, starting from a solution containing the microspheres, in which the solvent is allowed to evaporate slowly in suitable conditions. In this case, the driving force is capillary interaction, which originates from the deformation of the surface of a liquid caused by the presence of floating or submerged particles [15]. These two properties—weak interactions and thermodynamic stability—lead to the sensitivity to perturbations exerted by the external environment. Those small fluctuations alter thermodynamic variables.

Self-assembly also permits material structures far more complex than traditional metals, ceramics, and polymers, with many levels of hierarchical organization and compartmentalization typical of biological structures such as cells and organelles. Such materials may perform functionally in ways not possible today for traditional, non-biological matter. It requires developing simulation-based design tools that enable both the prediction of structures and their properties from building blocks and the rapid prototyping and reverse engineering of building blocks designed and pre-programmed to assemble into target structures.

A huge pool of a “bricks” of next-generation, self-assembled and self-programed materials are born enabling their self-reflection and self-direction within ingested collective intelligence. Nanoparticles and colloids of nearly any shape, made of metals, semiconductors, and/or polymers, and functionalized with organic molecules and biomolecular ligands—including proteins, viruses, and DNA—as well as other chemical “hooks” are now possible. The design space for self-assembled materials is now so vast that computational tools are required for the rapid screening and prototyping of building blocks that will predictably self-assemble into desired structures. In recent years, promising new theoretical and computational approach the study of self-assembly have emerged to guide experiments, but these are in their infancy.

At the same time, continued investments in high-performance computing (HPC) have produced computing platforms that are now fast enough to permit predictive simulations of self-assembly for complex building blocks, and new experimental probes promise the needed resolution of nanoscale structure to monitor assembly processes in situ, parameterize models, and validate simulation that might lead to marked changes in the structure and even compromise it, either during or after SA. The weak nature of interactions is responsible for the flexibility of the architecture and allows for rearrangements of the structure in the direction determined by thermodynamics. If fluctuations bring the thermodynamic variables back to the starting condition, the structure is likely to go back to its initial configuration. This leads us to identify one more property of self-assembly: reversibility.

One interesting example where authors cite number of hypotheses and mathematical models that try to explain how these structures self-assemble from liquid crystals is given in [16]. The authors were focused on liquid crystal self-assembly in plant cell walls (“nature’s most abundant biological fibrous composite”)—since this is an “energy-efficient material synthesis mechanism that plays a crucial role in building these materials with varied material properties”. One key term used in the paper [4] is plywood, describing the way in which self-assembled fiber constructions in nature are layered and oriented to produce particular properties—no matter whether the underlying biochemistry is based on proteins (collagen) and/or polysaccharides (chitin, cellulose) in animals or plants.

4. Computational science and PV cells

Here we explore the theoretical, experimental and technological challenges posed to organic polymeric and small molecules and inorganic nanostructure PV. A common feature of organic polymer and inorganic nanostructures is the localization of their excited excitation and carriers in bulk leading to the large electron-hole interaction [17], and consequently to an obvious fundamental issue – dissociation of excitation into separated electron and hole carriers. Beside excitation transport, single-carrier transport is another issue [6] since the hole has a very small mobility in the polymer, so the hole transport is very complicated and additionally there is an lack in understanding the description of the hole mobility: is it a hopping transport, or a free-carrier-like transport or tunneling transport.

Moreover, nanostructures pose a technology challenge on its own right in the areas of electronic structures, and electron-electron, electron-photon, electron-phonon interactions because of very sophisticated and

complicated nature of wavefunction localizations caused by quantum confinement effects, band offsets and piezoelectric effects. Further, Auger effect (electron-electron interactions) causes multiple excitation generation in nanocrystal and the effect can be further explored in order to achieve highly efficient solar cells. However as it is emphasized in [18] to fully exploit the electron-electron and electron-photon interactions in order to achieve the optimal efficiency of organic PV cells, one has to understand the carrier dynamics and possible quantum coherence effects and for it is needed to perform time-dependent simulations simultaneously for both the electron and atom. Computationally, and theoretically, this is very challenging. So the potential impact of computational science is huge and both, theoretical models and computational research can mutually benefit from each other, both supported with experimental verifications. One of the issues where impact of computing can be significantly seen is to find accurate and reliable way to calculate the wavefunctions and binding energies of excitations. The exciton is a bound state of an electron and an electron hole which are attracted to each other by the electrostatic Coulomb force. It is an electrically neutral quasiparticle that exists in insulators, semiconductors and in some liquids. The exciton is regarded as an elementary excitation of condensed matter that can transport energy without transporting net electric charge. The wavefunction of the bound state is said to be hydrogenic, an exotic atom state akin to that of a hydrogen atom. However, the binding energy is much smaller and the particle's size much larger than a hydrogen atom. This is because of both the screening of the Coulomb force by other electrons in the semiconductor (i.e., its dielectric constant), and the small effective masses of the excited electron and hole. The recombination of the electron and hole, i.e. the decay of the exciton, is limited by resonance stabilization due to the overlap of the electron and hole wave function.

Some of existing methods of calculating the wave function of exaction are as follows: variation wavefunction calculations, GW Bethe-Salpeter equation [19], excited–state quantum chemistry method [20], quantum Monte-Carlo method (which deals directly with the many-electron Schrodinger equation). However here is problem with scaling the simulation to size of the system since it requires pentascale computing or developing a new methodologies and parallel processing. Second issue is developing a good theoretical model which would describe and simulate atomic structure at the surface and interface. An initio molecular dynamics (MD) simulation seems to work well. However, to accelerate the development of a new generation of solar cells based on the organic polymers and nanostructure the supercomputer are necessity.

Another design of solar cells we want to mention here is based on biomimetic and hybrid technology which involves inorganic, organic and polymeric components interface with each other. Such structures are very complex, involving considerable challenge in reliable and effective predictions of the material structure and morphology stability, electrical transport, accurate predictions of level alignment in heterojunctions and contacts, etc. The reliable simulation of transport properties is necessity. One solution is dynamical simulations by using the Green-Kubo mechanism with the Boltzmann transport theory to calculate the thermoelectric power. Beside atomistic computational modeling technique there are important challenges such as development of force fields and coupled quantum mechanical/molecular methods for describing week (van der Walls) and strong interactions. To summarize the significant parallel computing and advanced modeling of transport properties and physical phenomena on quantum level are needed to accelerate hybrid technology for solar cell. New characterisation techniques help understand fundamental processes [21] where the major issue is electronic structure of heterojunction which heavily influences device performances and where major limitation of inorganic nanoparticles are related to the surface chemistry.

An interesting technique which was developed to study the properties of the silicon detector at LHC (CERN), so called the transient current technique (TCT) seems to be promising tool to study the photovoltaic solar cells [22-24]. TCT technique is suitable technique to study the charge-carrier transport mechanism. This includes the determination of electron and hole drift velocities as a function of electric field, charge carrier lifetimes as well as effective concentration of space charge in the sensor/detector bulk. The method is based on the injection of alpha source or laser short pulse close to surface and measuring the induced current in the detector electrodes as a function of time.

5. Computing the microgravity: Manufacturing in the space

The concept “zero gravity” is moved to the concept of “microgravity”. There are many surprises and not all experiment results have yet been satisfactorily explained. An early extensive study on microgravity effects on materials processing is given in [25]. Here we summarize some advantages that were enabled through microgravity: microgravity enhances the sedimentation and buoyancy, increases dopant homogeneity in semiconductors. Semiconductors are often doped to establish specific electronic properties (i.e. n-type or p-type). Convection on Earth can cause the distribution of these dopants to be inhomogeneous, degrading the

suitability of crystals for their intended application. Absence of convection [24] in microgravity enables uniform distribution of the dopants. Moreover microgravity expands the possibilities for container less processing. It enables accurate measurements of material properties such as viscosity and surface tension, facilitates nucleation studies, and increases the size of crystals that can reduce defect densities from contact with container wall [27].

6. Final remarks: Creating an innovating ecosystem

This paper provides learning opportunities for those who are not familiar with emerging trends in science of materials and computational science, both used as a driver force in the energy innovation sector. Importantly it gives an insight into innovations which are the results of a fruitful exchange of ideas among interdisciplinary research projects. It is enabled by an innovative ecosystem where approaches from different disciplines are transferred in the energy sectors (bio-mimicking in engineering such as the photosynthesis and self-assembling etc.). Doing extensive research on the trend of the emerging technologies we have the following conclusions:

- There is no single technology which would be a total solutions in itself;
- Developing an energy mix would become more important in the future;
- The current trends clearly addressing issues towards the integration of new technologies such as micro and nano-electronics, micro-and nano-electro-mechanical, micro-fluidic, magnetic, photonics, bio-chemical, multi-functional and smart integrated system;
- An understanding of technology fundamentals, prototyping at low scale, and then up-scaling and tech remonstrations are all very important in the development of new energy technologies;
- Technologies that aims at finding synergies of a wide mix of energy technologies becomes highly commended;
- Outcomes and approaches from research in fundamental science, such as quantum physics, particle physics and research in space should be significantly more implemented in modelling/simulation of material properties; particularly the techniques that are developed for the detection of defects in solid detectors (such as TCT techniques can be applied and further developed and advanced for the needs in the field of solar cells);
- An innovation in computational science education is of crucial importance in particular towards not only developing tools for verification existing tools but also towards creating new through accidentally merging the different concepts and by systematic studies of the outcomes;
- Developing curriculum at Universities with a wide mix of disciplines.

Achieving predictive capability will accelerate progress in Integration of synthesis, processing, characterization, theory, mathematical modelling, chemistry breakthrough discoveries and simulation. Simulation-based engineering and science benefit from predictive capability in science and engineering. Multimodal, multifunctional and multidisciplinary modelling has a significant role in accelerating scientific discovery, enabling new technologies, efficient transfer and incorporation of simulation-based engineering and science in industry.

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