International Research Journal of Engineering and Technology (IRJET) e-ISSN: 2395-0056
Volume: 07 Issue: 08 | Aug 2020 www.irjet.net p-ISSN: 2395-0072

Light-based Technologies and Materials Innovation: A Review

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Abstract - *Presents a good opportunity to reflect on the current and future impact of light based technologies and the role of physics in guiding that impact. For example, when we think of light and energy there are two approaches that come to mind: the here and now technologies (Si-based photovoltaics, solar thermal) and the "around the corner", high-risk, high-reward directions awaiting further development. A common link between both approaches is materials innovation and introducing new physics of light-matter interactions.*

Key Words: *materials innovation*, light based technologies, *Si-based photovoltaics, solar thermal.*

1. INTRODUCTION

Discovery of new materials: Predictive materials physics:In many ways, the light-based technologies in use today are limited by the performance of materials. This motivates the discovery of new materials, exploring materials physics of existing materials and exploiting new device concepts. Advanced materials share a common attribute: They are complex. Therefore achieving required performance depends on exploiting the many degrees of freedom of materials development including (but not limited to) multiple chemical components, nanoscale architectures, and tailored electronic structures. This introduces enormous complexity in the discovery process, complexity that must be understood and managed. A theory bias here would argue that we do not have the time or resources to explore all the options experimentally. However, our current computational methods confer upon us predictive power to accelerate discovery and innovation in materials. During the past decade, computer simulations based on a quantum-mechanical description of the interactions between electrons and atomic nuclei have had an increasingly important impact on materials science, not only in fundamental understanding but also with a strong emphasis toward materials design for future technologies. While the current theory tools are not perfect, they do provide sufficient information for theory-directed design of new materials and new materials physics. In addition to the computational design of materials for solar cells, artificial photosynthesis, and photochemical pathways to fuels, the need to computationally predict and optimize the light-matter interactions in materials is general and relevant to several light-based technologies including:

- Optical circuits
- Displays
- Solid-state lighting
- New light sources

A further link between established and to-be-developed technologies is that any new approaches must to some extent be integrable with dominant pervasive technologies and processes. This raises issues such as CMOS compatability and considerations of growth mechanisms, and on a more fundamental level the importance of both interface and volume effects in any new materials. This is particularly pertinent for nanostructured materials due to their increased surface-to-volume ratio. Hence, an adequate description of the physics occurring at interfaces of any new optoelectronic material must be taken into account in materials design and development from the start. In many cases, a single theory method or approach may not be enough. A strategy of multiscale simulations must be used to translate the results of atomistic calculations to real-world scales. Some aspects of this thesis (especially the chapters on ab initio plasmonics) illustrate the need and use of multiscale theory.

2. MATERIALS PHYSICS FOR ENERGY

Solar technologies, whether photovoltaic or solar-fuel based, are ultimately limited by the efficiency of the light absorber. One of the primary goals of this thesis has been to investigate new light capture and conversion strategies through materials discovery. Artificial photosynthesis imposes unique demands on the light absorbers, relative to conventional photovoltaics. In artificial photosynthetic devices, either a single material, or two absorbers arranged in a tandem cell format (and currentmatched spectrally), must at minimum provide the thermodynamically required voltage of 1.23 V to split water, and must provide comparable voltages to reduce CO2 to methanol or other fuel. However, very few Earth-abundant materials have been identified that have band-gaps in the 1.5-2.2 eV range and satisfy the requirements for photoabsorbers in a solar fuels device. This presents a unique opportunity for exploring new materials physics especially in context of wide bandgap semiconductors. Optoelectronic properties and relaxation dynamics of these wide bandgap semiconductors would find applications beyond artificial photosynthesis in solid state lighting and photovoltaics.

3. HIGH-THROUGHPUT THEORY

As shown in recent work by Ceder, Jacobsen, Norskov, and others, it is now possible to scan hundreds of thousands of possible combinations of elements across the entire periodic table, suggesting many new materials solutions that far exceed the traditional intuition of experts in these fields. Even incomplete and low-level theories have suggested novel combinations of materials for new energy technologies. In principle, finding the best solution to solar harvesting and other issues related to composition-dependent property optimization can now be accomplished using this approach. Experimental synthesis and screening efforts to match the throughput of such computational approaches are underway within the Joint Center for Artificial Photosynthesis and within othergroups. The challenges associated with high-throughput theory (and to some extent experiments) are picking the "level of theory" commensurate with the complexity of the material and the property being screened for.

4. OPTICAL PHENOMENA IN METALS: PLASMONICS

Prominent materials for photonic and optoelectronic components operating in the visible and near-infrared part of the electromagnetic spectrum comprise metals and semiconductors. Metals such as gold, silver, aluminium and copper are traditionally not materials of choice, due to their substantial absorption losses caused both by intraband and interband transitions. However, metals do provide a unique opportunity for photonics in this part of the spectrum, namely the existence of highly confined surface waves at interfaces with dielectrics. Here, the electromagnetic field can, under appropriate conditions, couple to the conduction electron plasma, setting up a hybrid mode, termed surface plasmon. For extended interfaces, propagating modes with mode areas below the diffraction limit are possible (surface plasmon polaritons), whereas metallic nanostructures act as optical nano resonators with minute sub-diffraction-limit mode volumes (localized surface plasmons). The last two decades have seen an explosion of interest in surface plasmons, and a distinct research area of photonics, termed plasmonics, has emerged. This resurgence of interest in metal optics was to great extend facilitated by rapid advances in nano fabrication, near-field optical detection techniques, and computational modelling techniques taking the dispersion of the metal into account.

The high mode confinement that surface plasmons offer is made possible by a substantial penetration of the electric field into the metal itself, increasing with frequency until the surface plasma frequency is approached. This leads to unavoidable absorption losses and hence to a trade-off between localization and loss, which has hampered widespread applications of plasmonic waveguides and nano resonators for applications in integrated photonics. However, over the past few years it has been recognized that the optical losses also provide unique opportunities: Firstly, short dephasing times of only a couple of femtoseconds allow, under appropriate circumstances, for substantial emission enhancement of nearby (low internal quantum efficiency) nanoemitters. Secondly, decay of surface plasmons via absorption creates electron/hole pairs, and if these hot carriers can be harvested before thermalisation applications in hot carrier photodetector, catalysis, and nano chemistry seem.

5. OPTO ELECTRONICS AND NANOPHOTONICS

The potential for an order of magnitude improvement in size reduction of optoelectronic devices facilitated by plasmonic sub-diffraction-limit light confinement has intrigued researchers over the last decade. This directly addresses both the size mismatch between current electronic and photonic components, and furthermore promises substantial increases in modulation/switching speed, and potentially also lower energy consumption. Yet as described in the previous section, the unavoidable optical loss inherent in plasmonic light localization has to great extent hindered technological adoption of this approach. Since the physical limitations and parameter space for localisation and loss in plasmonic waveguides and nanostructures are well understood, focus has shifted to work on the underlying plasmonic materials for further improvements in performance. On the one hand, for

the dominant plasmonic materials gold and silver, a substantial amount of research effort has been put into achieving higher crystallinity and hence less domain- and surface-induced optical losses. Examples include self-assembled-monolayer-assisted thin film growth for smoother films or backetching of silicon in silicon/noble metal multilayers in order to expose an essentially single-crystal surface layer. At the same time, there is an active search for new plasmonic materials particularly in the near-infrared part of the spectrum underway. Here, materials with improved temperature stability such as TiN are attractive for applications such as Heat-assisted Magnetic Recording (HAMR), and also from the viewpoint of CMOS compatibility. Other candidate materials for applications in the near-to-mid-infrared are highly doped zinc oxides or perovskite-based ferroelectrics. Apart from the physical properties plasmonic materials in isolation, it is also necessary to gain understanding and control over the materials physics at interfaces, particularly if both photonic and electronic phenomena associated with highly concentrated optical fields are to be exploited.

Examples include plasmon-enhanced carrier transfer in Schottky-type photodetectors, or metallic nanostructures coated with molecular overlayers for catalytic applications. It is in all these areas that improvements in materials deposition and multilayer assembly go hand-in-hand with predictive theoretical studies enriching both

our understanding of the underlying physics, and guiding further improvements. The employed methods necessarily are inherently quantum in nature, in contrast to the mainly classical modelling of plasmonic devices solely exploiting optical effects, which is firmly

6. CONCLUSION

The underlying theme of this thesis is exploring light-matter interactions, from a joint theory and experimental standpoint, in the context of high-risk, high-reward microelectronics and nanophotonic technologies. This work is motivated in part by the materials-based challenges in current devices and in part by the search for new phenomena to enable novel microelectronics and nanophotonic devices. First part of the thesis presents the work my collaborators and I have done on Zn-IV nitrides, an example of theory-directed functional materials design. The second half of the thesis presents our work on ab initio calculations for plasmon decays and dynamics of hot carriers with a focus on understanding optical phenomena in metals.

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