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Research domain(s), discipline(s)/sub-discipline(s)

Materials Science

Title of Response

Enhancing CMOS interconnections

Abstract

We enable CMOS computing to interface to optical systems rapidly and with direct interconnections.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

Optical computing interconnections that enable existing computing systems, cloud computing, and computer server farms to run faster with less energy consumption is the next step in the future of CI. This is true for all types of applications and disciplines. The backbone of optical-assisted computing and, in fact, all optical computing (AOC) and optical CI, will be devices made with fast, efficient electro-optic (EO) materials. We are committed to designing the best CMOS-compatible electro-optic material that will, in one step, encode information from a processor to an optical output that can then be used by a local processor or even to a distance memory unit. Our current work has already demonstrated that our modeling has allowed us to design and synthesize EO materials that have four times the capability of current state of the art materials. Our research further shows that it is theoretically possible to find materials that will perform two orders of magnitude better than what now exists. The process of finding such materials requires extremely large data sets and the simultaneous computation of many parameters. AI is required to identify the emergent properties of these large sets of potential molecules to identify those with the best chance to be synthesized and simultaneously have the best chance at being highly efficient EO materials. This data-intensive computer modeling significantly streamlines the entire process of finding and synthesizing EO molecules that are increasingly efficient.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

In the initial steps of designing EO materials, we need access to a large enough array of computers with sufficient storage space to ultimately be able to simulate on the order of 1 to 10 million molecules. During the process of data acquisition, (which is the output of the computation) we will need AI specialists, with machine learning tools, to identify the emergent properties of the molecules to target new molecules that will have a higher chance of being better EO materials. Determining if these candidate molecules can be synthesized will require organic chemists using existing, costly tools of retro-synthesis which will be integrated into our methodology. Then, once molecules are made, we need to evaluate their potential as EO materials, and adaptability to the interfaces required by CMOS circuitry. This requires both statistical mechanical simulation of such materials at the interface, and the ability to simulate the effects of interfacial materials on the EO materials (to improve their order and compatibility with the existing devices) and the nature of the electric and magnetic (E&M) fields generated during the interaction and the conversion from electric to optic signals, all of which requires statistical mechanical and E&M theory. These are large scale problems with hundreds to thousands of molecules that require large computing facilities with large data storage. Solving the issues of structural morphology at interfaces when large electric fields are present is only in its nascent stages, and is the next major challenge to quantum based and multi-scale theory.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

The process of moving from the conception of a new EO material to the integration of that material with CMOS compatible components is a long one that requires a number of steps, as described above (molecule design, synthesis design, synthesis, initial testing, interfacial adaption, testing in devices and scalability, reproducibility, and finally a marketable device.) This effort requires a team, with each member an expert at one aspect of the problem. Each step should be comprised of a well-integrated team of theory/modeling experts, a synthetic chemist and a characterization specialist. The challenge is to bring all of that to focus on a single problem. The most efficient structure is a grant to a single PI or a few PIs (working in close concert) with sufficient resources to bring in theoreticians, experimentalists, materials interface experts, AI experts, and Machine Learning experts to handle the ultimate integration problem at each step along the way.

-- End Submission –