## A Proposal for Materials Sciences IT faculty hires in Chemistry

## I. Introduction

We are proposing that information technology initiative funds be used to hire faculty engaged in state-of-the-art materials research relevant to information technology (IT). While the details of the information technology initiative are still emerging, it is clear that modern materials research with potential industrial connections will have chemistry-based efforts at its core. There are some clear issues that will persist as driving forces as the details of the initiative are clarified. With this in mind, the Department of Chemistry proposes future hires that will be linked to clusters that are yet to be formed. The Department of Chemistry can play a major role in the IT initiative in many different ways. It should be noted that materials processing and development play key roles in the IT industry, and the Department of Chemistry can provide key contributions in this regard. We suggest chemistry faculty hires that will play a key role in such research clusters. We are actually proposing two related materials science faculty hires, one in theoretical chemistry and the other in experimental chemistry. As examples of the types of hires we envision, we give two example hires: a theorist with expertise in an area related to processing issues, and an experimentalist with expertise in nanomaterials development and characterization. Both areas are extremely strong with respect to potential economic development activities, and both are also well suited to a natural integration into the existing university strengths that characterize ongoing research at LSU. This is extremely important as it allows us to accomplish the goals of the IT initiative while capitalizing on the considerable existing strengths of the university.

### **II.** Rationale

There are several reasons for materials research to be a unifying theme for the information technology effort. First, materials development can have a major economic impact, particularly via patent activity. Secondly, there are considerable strengths already present at LSU in materials research. Thirdly, it is an area where we can recruit quality faculty with relative ease. The chemistry department will have at least two ways in which it can assist in the development of research clusters at the university. First, it is likely that there will be a nanomaterials focus, and secondly, there probably should be a focus on semiconductor processing. Both of these efforts can and should include chemistry efforts, both because they will build on historical and current strengths of the university, and secondly, because such research naturally dovetails with the plans for cutting edge research that can be coupled to growing economic engines in the state. Moreover, the ideas that we propose here will include multidisciplinary efforts by the Colleges of Basic Sciences, Arts and Sciences, and Engineering.

#### A. Nanomaterials - experimental

Let us first consider the case of an experimental hire that would emphasize novel nanomaterials. This is an area ripe for expansion, and we have an excellent opportunity to hire true "stars" in this area, based on the recent build-up of high-quality faculty in recent years.

Certainly, the chemistry department has had a strong effort in such nanomaterials efforts in the past (e.g., synthesis research of Strongin, nanoparticle preparation of Spivak, thin films activities of McCarley, guest-host chemistry of Warner, dendrimer development of Newkome, and ongoing efforts by recent hires such as Profs. Julia Chan and Gudrun Schmidt). Some appropriate high-visibility hires could obviously kick up the level of effort to the point that we could be true international leaders in such efforts. Moreover, such efforts naturally incubate multidisciplinary activities. We would likely interact with the Departments of Physics and Astronomy, Mechanical Engineering, Chemical Engineering, and perhaps several others. The key point is that new materials synthesis, design, and characterization is done by chemists. It is worth noting that buckyballs were discovered by experimental physical chemists (Nobel Laureates Rich Smalley from Rice University, in collaboration with Harry Kroto and Bob Curl). Moreover, the current research thrust in nanoelectronics is led by experimental chemists, including Jim Heath of UCLA, Stan Williams (currently of Hewlett Packard, previously at UCLA Chemistry, as well), Charles Lieber of Harvard, Paul Alivasatos of UC Berkeley, and a host of others. Finally, it should be noted that such research activities dovetail with economic development efforts, both directly in the short-term, and also in the long-term time frame. Industrial leaders, such as IBM, Hewlett-Packard, and many others are emphasizing new nanomaterials development including "buckytubes" as nanoconductors and nanoswitches, nanoparticles (i.e., IBM's "Magic Dust") for higher density information storage. Note that these are only examples of how experimental nanoscience chemists can contribute to IT initiative. A closely related, and equally important area is the growing effort in molecular electronics. The opportunities are considerable, and experimental chemistry has a strong role to play. Experimental chemists have been leaders in this effort, and we propose that hires in this area at LSU will allow us to participate in these activities in natural and beneficial ways.

We propose this as an area of focus for the IT initiative. LSU already has some efforts designed to study nanomaterials and the additional hires will complement and enhance this effort. Specifically, we propose to hire experimentalists specializing in the preparation and analysis of clusters ranging in size from a few tens of atoms to hundreds or more atoms. This is a portion of the nanoscale field that is not represented at LSU, but would complement the efforts of many LSU faculty in Chemistry, Physics, and Engineering.

## B. Electron scattering theory (theoretical plasma processing)

Microfabrication methods are of critical importance to the semiconductor industry, as evidenced by much of the work around the nation and at CAMD. Improvements in techniques require a close interplay between experiment and theory. The data generated by electron scattering calculations are a critical component in the development of more powerful simulation tools for the plasma processes and reactors used in microelectronics fabrication. Indeed, major industrial giants such as Intel fund such work, and it is expected that there would be multiple benefits to faculty hires in this area. Obviously, there is the possibility of additional industrial interactions, both collaboratively and through industrially financed, LSU-based research. This type of interaction is the basis for local economic development over the longer term, and fosters additional research funding even in the short term. Secondly, the calculations can exploit highperformance computing provided by massively parallel computers to study electron-impact dissociation of polyatomic molecules into reactive fragments for gases relevant to the plasma processing steps in semiconductor manufacturing. Thus, computing expertise at LSU would be enhanced by such university-based efforts. Indeed, such computational scientists would complement ongoing research efforts in the College of Basic Science (particularly the Departments of Physics and Astronomy and Computing Science), as well as the College of Engineering (especially the Departments of Mechanical Engineering, Electrical and Computer Engineering, and Civil and Environmental Engineering). This IT project offers an opportunity to apply high-performance computing to meet a technological need and a challenging incentive to explore collision processes about which little is known. Thus, we propose the hire of a faculty member whose research focuses on the relevant issues in molecular scattering theory.

# **III.**General considerations

Both of the areas listed above will serve important and far-reaching objectives that are central to the IT initiative effort. They will allow LSU to advance in important scholarly activities, capitalizing on existing strengths while creating new ones, and also provide fuel for economic growth in fundamentally new and important ways. First, the research that will be performed is relevant to the high-technology IT community currently, as evidenced by the fact that industry currently subsidizes such research. Secondly, the research fostered by the IT initiative will likely result in successful patent applications, and the Department of Chemistry has a good track record of pursuing such efforts. Thirdly, faculty with expertise in the materials efforts noted above will better prepare students to enter the modern, IT-intensive workplace. As is always the case, good faculty will train good students, and the Department of Chemistry has an excellent track record of attracting internationally competitive talent. It is anticipated that the luster of the IT funds will allow us to continue, or even enhance this hiring track record. Indeed, such efforts will allow us to initiate a "snowball effect", whereby the new faculty will nucleate a variety of interdisciplinary activities. It is anticipated that such faculty members in the Department of Chemistry will also be good partners and collaborators with IT faculty hired in other departments. Indeed, the Department of Chemistry has frequently fostered high quality, multidisciplinary research in the past, and the availability of IT funds will permit similar activities, albeit on a grander scale than in the past. This is an excellent opportunity for the Department of Chemistry and the university and economic community as a whole.