RESEARCH PLAN

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Research Objectives

The overall objective of my research is to apply the methods of statistical mechanics and computational physics to various nanoparticle systems. Such nanoparticle systems are expected to become basic elements of many novel advanced nano-structures and nano-devices. The results of my research will permit analysis of numerous new experimental results on nanoparticle systems, and also to make predictions about physical and chemical properties of these systems.

Overview of the Field

Metallic nanoparticle science has a long history. For example, a ceramic cup known as the Lycurgus Cup, which dates from the fourth century AD, has long been known to have very unusual optical properties, which has been clarified by a recent transmitted electron microscopy (TEM) study that these properties originate from the accidental inclusion of nanoparticles in the cup material. In the modern era, very tiny particles have been used systematically in photography, catalysis, and stained glass.

The current nanoparticle research aims at the creation of functional materials, devices through control of structure on a nanometer length, and thus differs from the older uses of nanoparticles in several ways. First, very accurate manipulation and systematical organization of nanosize materials now become possible. Secondly, new technologies for the study of nanoparticles tend to be highly interdisciplinary, due to the varieties of the involved materials and techniques.

Here I briefly introduce some examples among these new technologies, within the limited scope of the relation of my future research studies:

- Synthesis of nanoparticles with accurately controlled size and shape: Such synthesis allows for novel applications, such as the creation of a single layer of nanoparticles, and highly controlled catalysis.
- Use of chemical techniques to attach molecules such as proteins or DNA to nanoparticle surfaces: Related to these techniques is dip-pen nano-

lithography, with which one can deposit nanoscale patterns of chemical compounds onto a substrate.

- Fabrication of linearly aligned nanoparticle chains, with a manipulation by atomic force microscopy or electron beam lithography. These methods can accurately control the position and size of nanoparticles.

Also these techniques are being developed very rapidly, and the accuracy of them and the number of materials which can be manipulated by them increase very rapidly. Novel applications using them are proposed intensively. Here I present a list of these applications, again in the limited view of relation to my research plan.

- DNA sequence detection or diagnostic bioassays using the electronic or optical properties of DNA conjugates such as DNA/gold nanoparticle composites, DNA/polymer nanocomposite;
- Programmed nanoassembly of nanostructures such as photonic crystals, based on the properties of the surrounding molecules, bounded on the surface of the nanoparticles;
- Surface plasmon applications (known as "plasmonics"), such as energy transfer of light in the smaller scale than the diffraction limit in linear chain of metallic nanoparticles, biodetection using surface-enhanced Raman scattering, and fabrication of nanolenses through suitable arrangements of nanoparticles;
- Advanced drug delivery systems using chemically modified nanoparticles.

One thing I hope to emphasize here is that for the development of above nanotechnologies, the disciplines of statistical mechanics and computational physics can play a major role. Current nanoscience and technology try to combinationally use very different materials such as chemical materials and metallic nanoparticles. In this circumstance, statistical physics is essential since it provides deep conceptual insights in fields such as chemical engineering, physical chemistry, and condensed matter physics; these insights can lead to new, predictive capabilities in nanoscience. Computational physics is also obviously crucial, since the techniques from it are indispensable to calculate physical and chemical properties of the advanced materials in nanotechnology, and to make predictions about whether newly designed nanostructures such as smart drug delivery system made of these advanced materials will be functioning or not.

Research Plan

My planned research involves several distinct but related in theoretical nanoscience:

- **Phase Transitions and Structural Formation in Gold/DNA Nanocomposites**

I will continue to study phase transitions and related phenomena in DNA/gold nanocomposites. This is a system which consist of an aqueous suspension of gold nanoparticles and DNA strands. Depending on conditions of preparation, such as temperature and salt concentration, this system may exhibit a variety of phases.

In a recent paper, I have proposed that two different types of phase transitions can occur in this system: a melting transition, where the DNA/gold aggregate breaks up into isolated particles in suspension, and a sol-gel transition, at which the DNA/gold aggregate changes its morphology from a fractal gel to a compact sol. The melting transition is related to DNA dehybridization, but is much sharper in temperature than that of the single DNA strands. This characteristic is very important in applications to DNA detection, since this feature provides enough resolution to optically or electrically distinguish perfectly matched DNA pairs from matched pairs but with some defects. The sol-gel transition is also very important for chemical processes used to make thin films or well-ordered materials. Moreover, the knowledge of the existence of gel structure can lead us to better improvement of biosensing application like biobarcode methods: In the barcode method, a gel structure can provide high loading of barcodes, and can be used as a unique universal magnetic nanoprobe.

In order to investigate physical properties of this system, I have developed a structural model to describe the morphology of the system at given temperature, using *statistical mechanics*, and then have calculated the optical properties of this system, such as the extinction cross-section, by using the so-called Discrete Dipole Approximation calculation. Since this model can describe both the structural and the optical properties of the system considerably well, I will extend it to similar systems like DNA-polymer nanocomposite or DNA-dendrimer systems.

In addition to this, I am also planning to investigate the *mechanical* and dynamical properties of this system, using Molecular Dynamics (MD) techniques. However, there are many practical problems to directly apply MD calculation to this system, since we should consider different types of materials at once. Thus, in order to circumvent this problem, I plan to construct efficiently simplified model for this system using statistical mechanics. This type of study is closely related to my third research proposal, so I will discuss more detail of this modeling later.

• Surface Plasmon Optics in Well-Aligned Array of Metal Nanoparticles

As another project, I will investigate surface plasmon application of aligned metal nanoparticle systems, using computational physics techniques. Recently, applications of surface plasmon optics in nanoscale metallic systems have developed rapidly. These include energy transfer through ordered one-dimensional arrays of nanoparticles, surface enhanced Raman scattering, nanoantennas, SPASERs (Surface Plasmon Amplification by Stimulated Emission of Radiation), and nanolenses, to name just a few.

I will investigate surface plasmon transfer in linear arrays of metal nanoparticles. In the well-ordered structure, the surface plasmon of individual particles can couple each other to form a surface plasmon band structure. This surface plasmon band structure of such linearly aligned metallic nanoparticles is analogous to the electron band structure of solid. States in this band structure can absorb incident light and transfer the energy to a surface plasmon which can propagate through the nanoparticle chain. This mechanism permits transfer of light energy below the diffraction limit, where a conventional waveguide or photonic crystal cannot guide a wave.

When the distance between the nanoparticle centers is greater than about three times their radius, the surface plasmon dispersion relation can be obtained using the dipole approximation. However, if the separation becomes smaller than this value, the interaction between nanoparticles becomes stronger and multipole contributions become important. My recent paper shows that, for spherical nanoparticles, the surface plasmon dispersion relation can be obtained exactly taking into account a certain electromagnetic pole spectrum of this system. However, for more general nanoparticle shapes, which may be important in practical applications, this analytical approach may not be applicable. Under these conditions, numerical treatments, such as the finite difference time domain (FDTD) approach or the discrete dipole approximation (DDA), are necessary. In order to treat these applications, I will study this system using the FDTD technique in order to solve such problems such as determining optimized shape of nanoparticles, and optimized distance between the particles for such applications.

Other applications of this system become possible by using anisotropic or nonlinear materials. For example, if the host of this system is a liquid crystal (LC), which has anisotropic dielectric properties and a principal dielectric axis of which can be controlled by an external electric field, the surface plasmonic properties of this system can change depending on the direction of the external electric field. For example, in the recent experiments done by German researchers, they demonstrated that the surface plasmon frequency of a LC-coated nanoparticle can be controlled by an external electric field. In my recent paper, I theoretically showed that this method could indeed produce a measurable change in the SP frequency. Moreover, in a paper submitted to Phys. Rev. Lett, I've also found that the deformation of LC director near the surface of a gold nanoparticle, which was presumed to hinder the change of the SP frequency, can surprisingly enhance the change in the SP frequency of a LC-coated nanoparticle. Thus this result indicates that electrical control of surface plasmon transfer of one dimensional metallic nanoparticle can also be possible. I will continue to extend my work to such materials in this direction.

In summary, surface plasmon nano-optics is an exciting new field which promises many interesting new applications which demand major computational efforts for the efficient design of useful new materials. I will continue and extend my present work in this newly emerging area.

- **Computational Studies of Chemically Modified Nanoparticle Systems**

I will investigate gold nanoparticle composites containing various molecules. The method currently used to attach DNA sequences to the surface of gold nanoparticles can be extended to other chemical compounds, such as proteins, enzymes, etc. There are already several ongoing projects worldwide, using gold nanoparticles in an advanced drug systems to treat cancer. For example, a research group at Rice University uses a gold-coated nanoshell, in which cancer-specific antibody proteins are embedded, to selectively destroy cancerous tumors. A joint U. S.-Netherlands research team is using colloidal gold nanoparticles to deliver an anticancer protein known as tumor necrosis factor (TNF) directly to the tumor without serious side effects. Moreover, there are many research proposals to develop a way to load nanoparticles with a variety of useful chemical compounds, such as drugs and detector molecules, in order for this complex material to work as an advanced pharmaceutical system. For example, a research group in Georgia Tech synthesize magentic nanoparticles with cancer killing drug and a receptor which can initiate a receptor-mediated endocytosis, and by which these complex structures can selectively enter into targeted cancer tumor cells. However, there are many obstacles which prevent these complex materials from achieving their originally designed functions. For example, in case of DNA/gold nanoparticle system, when sodium concentration in the solvent is too high, the DNA strands which are attached to the gold nanoparticles attract sodium ions, so that local sodium concentration near the gold nanoparticle surface is higher than the average. This effect leads to collective melting of the DNA strands near the surface of gold nanoparticles. And in case of the magnetic nanoparticle-based drug systems which were proposed by a research group in Georgia tech, the percentage of nanoparticles entering into cancer cells by receptor-mediated endocytosis, is very low. This may be caused by the deformation of receptor conformation due to different environments around the surface of nanoparticles, as seen in DNA/gold nanoparticle system.

An economically efficient way to verify whether newly designed complex materials will work as originally proposed, should be computer simulations, such as molecular dynamics approaches. However, since these systems are very complex, direct simulations may not be possible with current computing power. To overcome this problem, it is advisable to develop an effective model for each component of this system, using a statistical mechanical approach. In this direction, I am working on a project to determine equilibrium structure of a single DNA strand which is attached on the surface of gold substrate in an ionic solution. In this case, we can simplify an ionic solution by using Possion-Boltzmann equation, and also we can treat a gold nanoparticle surface as a flat conductor surface, so that we can consider the contribution of electrons inside the gold surface for a charge by using an image charge method. As we can see in this project, we need various simplified models to consider the contributions of different objects inside a newly developed nanoparticle-based drug delivery system. Also we need many efficient computational algorithm to deal with the system within reasonable computation time, since the system should be big enough, in spite of the usage of many simplified models. Thus, as a long term project, I will perform a computational study of this drug delivery system by developing efficient computer simulation techniques and effective statistical models.

Required Equipment

To successfully carry out this research plan, a Linux-based PC cluster, or similar cluster, will be needed. By now, it is a routine task to build a Linux-based PC cluster. Such a cluster is the best way to obtain high performance computing at a rather economical cost. Moreover, this type of system is suitable for applications which are not communication-intensive but which require great computing speed and very large memory. These are the applications which I envision in my planned research.

My background is ideally suited for this type of computing. I have great experience in numerical studies using high-performance computing. I also have ample knowledge of both constructing and managing computer systems, which I acquired when I was a computer assistant in the physics department as a graduate student at Seoul National University. With this experience, I will be able to construct a high-performance Linux-based PC cluster and to carry out my planned research projects using this cluster.

Cooperation with Other Groups

The research plan which I propose here is highly interdisciplinary and deals with many different types of materials. Thus, cooperation with other research groups will play an essential part. Currently, I am collaborating with the Stroud group at Ohio State University, the Schatz group, two experimental groups (Mirkin and Nguyen group) at Northwestern University, and the Joannopoulos research group at MIT. I plan to seek further collaborations with other research groups as well.

Philosophy and plan of teaching

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The most important aspect of teaching physics nowadays is giving a motivation to students. In my opinion, this motivation can be given to them by letting them know what we can eventually do using physics. Although this goal is the same in all the level of the student, the method can be different. Moreover, in any case, fun should be involved in this process.

To achieve the above goal, I plan to develop new courses for both undergraduate and graduate level. For undergraduate students, I hope to stress on teaching scientific reasoning rather than physical knowledge. Thus, I plan to let them know how important scientific reasoning is and how we can use this scientific reasoning to deduce new knowledge from the known facts. This can be easily done when we explain the things happening in the real world with physical concepts, for example, when we explain the relationship between the effective defensive formation in football and the concept of linear momentum conservation or when we explain Michael Jordan's airwalk in the concept of central mass. In this direction, I plan to develop new introductory courses like "physics in real life". Also this kind of teaching method can be extended to the more advanced level course for undergraduates such as quantum physics, thermal physics, statistical physics, and computational physics. In a long-term project, I plan to develop such courses.

For graduate students, I think that motivation can be given by explaining where the frontier of physics lies in, or how we can connect what we teach to them with the current research topics or novel applications. We can setup the course to incorporate with the current development Thus I plan to setup the course in the way to fit the direction which I explain. In this direction, I plan to develop the course of theoretical approaches for nanotechnologies, computational physics, statistical mechanics in which I hope to emphasize the applicability of statistical mechanics not only to physical systems but also to many fields such as biological or chemical systems.