Breast Cancer Screening:

It is highly desirable to develop a non-invasive procedure using artificial intelligence techniques (AI) that can detect and reliably interpret images and data from small volumes of the breast. Over 240,000 women have been diagnosed with breast cancer in 2015, and the consequent need of an accurate, early diagnostic tool should have a significant impact on women's health. We propose using Artificial Intelligence [AI] techniques coupled with ultrasound, to develop *in vivo* methods of breast diagnosis to look for potential malignant tumors. A successful previous study was performed using *in vivo* P-31 Magnetic Resonance Imaging (MRI) in which we demonstrated a correlation between the MRI spectra and the type of breast tumors present in test subjects. However Magnetic Resonance Imaging (MRI) scans are expensive, especially P-31 MRI's which would require modification of current machines. We believe with current technology available from ultrasound scanners, a much earlier diagnosis and detection of potential breast tumors can be accomplished. The combination of this scanning method and AI techniques should provide a wealth of data capable of making distinctions between malignant and non-malignant breast tumors. This should have the enormous effect of reducing the need for potential needle biopsies and/or exploratory surgery, both being very expensive and usually requiring potential hospitalization. In addition, the current method of screening breast for cancerous tumors is a mammogram, requiring expensive x-ray equipment and requiring women to travel to a clinic or hospital. The great advantage of using ultrasound is that it is relative inexpensive, easily transported and requiring much less technical expertise. In rural locations or in countries where travel to medical facilities is difficult, the ultrasound equipment could be brought to women easily and quickly. Ultrasound is also much safer than x-rays and could be performed more frequently without concern of radiation exposure.

Parkinson's Disease Project:

Current therapies to treat Parkinson's disease are based mainly on replacement of dopamine within the striatum by medications like L-3,4–dihydroxy phenylalanine. Effective neuroprotective strategy for Parkinson's, to halt or slow down the dopaminergic neurodegeneration is yet to be developed. Maintaining alpha-synuclein in the native and soluble random coil conformation, and consequently preventing alpha-synuclein neurotoxicity could provide effective therapy on a molecular level. Recent evidence from *in vitro* and *in vivo* studies indicates that heat shock proteins are potent suppressors of neurodegeneration and are therefore promising therapeutic targets for neurodegenerative disorders (Sherman and Goldberg 2001; Muchowski and Wacker 2005).

Our artificial neural network (ANN) is a type of artificial intelligence consisting of an interconnected group of artificial neurons that uses a mathematical model or computational model for information processing based on a connectionist approach to computation. Our results are usually considered accurate to within 95% predictability. The software we use is *Nets* and was designed by the Artificial Intelligence Division, at NASA Johnson Space Center in Houston.

In this project, an ANN will be trained using molecular orbital energies of the 20 lowest unoccupied molecular orbitals (LUMOs), 20 highest occupied molecular orbitals (HOMOs) and dipole moment as input layers and the IC_{50} (minimum concentration of a compound fatal to 50% of the test population) values for Geldanamycin (GD). It is our objective to develop new drugs which can provide derivatives which will inhibit Hsp90 and significantly improve the treatment of Parkinsons disease.

Modeling studies for hydrogen fuel storage:

Atomic cluster materials at the nanoscale dimension have unique properties distinct from the bulk phase. There is a huge need for a fundamental understanding of the relationship of the properties of small nanoclusters and the bulk chemical and physical properties of metallic atoms combined into various small nanomaterials. These studies are expected to lead to an understanding necessary to design, model and synthesize materials which will exhibit the specific bulk macroscale property of storing hydrogen for use as a future fuel in a hydrogen economy.

Hypothesis: There is a determinable correlation using artificial neural networks (ANN) between the *ab initio* SCF-MO/DFT determined energies of orbitals of small metallic and alloy clusters, and, the bulk physical property of hydrogen uptake in a corresponding macro-scale system.

Computational Methodology:

The "holy grail" of computational materials' science would be to have the ability to accurately predict the chemical and physical properties of materials from a limited set of known parameters. Although there are many empirical and quasi-empirical methods available, there is no single method available which can perform this task in general, and especially from first principles. We have developed a procedure using an artificial intelligence method of neural networks, which has been used successfully in our center, to predict various physical and chemical properties of molecular and biomolecular systems.

A main goal of this research is to study and to develop new families of alloys that can reversibly absorb large amounts of hydrogen. The preparation of the alloys was done by starting from the composing metals weighted in the corresponding ratios to the formula that is desired. When these modeling studies are complete, we should have an excellent idea of the materials which can store large quantities of hydrogen gas safely and at temperatures and pressures which are safe and inexpensive.

Alzheimer's Research:

Alzheimer's disease (AD) is an irreversible neurological disorder, progressive brain disease that slowly destroys memory and thinking skills. Alzheimer's is the most common form of dementia, a general term for memory loss and intellectual abilities serious enough to interfere with the daily activities. Genetic factors, lifestyle and environmental factors play a crucial role in the onset of Alzheimer's and its progression. Alzheimer's disease (AD) is caused by the formation of the Amyloid β protein plaques and fibrillar structures in the brain. Protein aggregation is the most important factor that causes most of the neurodegenerative disorders such as Alzheimer's, Parkinson's, and Prion diseases. Given the high risk and pervasive nature of AD, there is a consequent urgent need for a highly accurate, early diagnostic tool to detect AD at a very early stage. This project will have a significant impact on the understanding of the disease onset and progression in patients suffering from AD. This study will address the long term effects of the injuries to the brain on chances of occurrence of AD. The novel research effort of this project will help and aid in the early detection and disease progression of Alzheimer's, and impact the diagnosis process of AD. This study will also address the diagnostic technologies, incorporating the Genomics/Proteomics/Bioinformatics approaches. It is proposed that different modeling procedures of Artificial Intelligence (AI), will be used in the areas of early detection, including Artificial Neural Networks (ANN), Adaptive Resonance theory (ART), etc. which can be used to detect patterns in AD patients that can provide a confirmatory diagnosis of patients with Alzheimer's disease.

Myeloproliferative Disorders

Myeloproliferative disorders is the name for a group of conditions that cause blood cells, platelets, white blood cells, and red blood cells, to grow abnormally in the bone marrow. Though myeloproliferative disorders are serious, and may pose certain health risks, people with these conditions often live for many years after diagnosis. The prognosis largely depends on the type of disorder. Myeloproliferative disorders include:

Polycythemia vera. Occurs when the bone marrow produces too many blood cells, especially red blood cells. More than 95% of people with polycythemia vera carry the blood mutation JAK2V617F.

Essential thrombocytosis. Occurs when the body produces too many platelet cells, which help blood to clot. Clots can block blood vessels leading to heart attack or stroke.

Primary or idiopathic myelofibrosis, also known as myelosclerosis. Occurs when the bone marrow produces too much collagen or fibrous tissue in the bone marrow. This reduces bone marrow's ability to produce blood cells.

Chronic myelogenous leukemia (CML). Cancer of the bone marrow that produces abnormal granulocytes, a type of white blood cell, in the bone marrow.

The emphasis of this work will be to define interactions between the protein molecules involving blood cells and drug molecules. The idea will be to develop drugs which can modulate the production of excess blood cells, either platelet cells, red blood cells or white blood cells. If molecules could be found to modulate these blood cells, it may be possible to control through medication, this overproduction. If suitable drug molecules could be developed, it may be possible to control these disorders similar to the way daily additions of insulin can control diabetes.