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## **COMPUTATIONAL MATERIALS MODELING**

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### **ABSTRACT**

Functional materials are designed to perform specific functionality. Their chemical and physical properties are sensitive to a change in the environment such as electric field, magnetic field, optical wavelength, and temperature. These materials yield usable chemical, electronic, optical, magnetic, transport, thermal and mechanical properties. Functional materials cover a broad range of materials, such as stimuli responsive materials (piezoelectrics, ferroelectrics, shape memory alloys, electroactive, magnetostrictive materials, electroactive polymers etc.). Metallic nitrides, high performance ferroelectric materials, magnetic shape memory alloys (MSMA) and stress corrosion cracking in metals have been investigated. Density functional theory (DFT) has been used to understand behavior and properties of these materials as a function of chemical constitution, composition, and structure for improving their performance for engineering applications. Ground state and response (electrical, mechanical, optical and magnetic) properties of functional materials have been investigated. Equation of state (EOS), lattice dynamics (Born effective charges, static dielectric constants, phonon band structures and free energy), elastic constants, and magnetic moments are some of the important properties that have been calculated.