The Physics Department of the University of Wisconsin-Madison

John H. Van Vleck Lecture

W.Y. Ching

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Application of Orthogonalized Linear Combination of Atomic Orbital Methods to Complex Materials

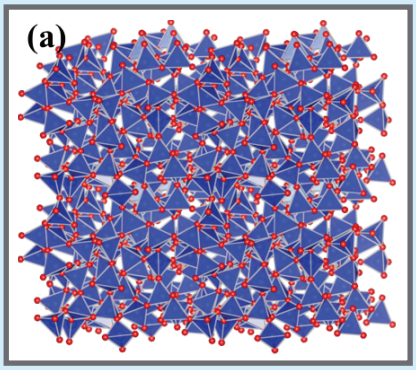

Figure 1

In this lecture, I present the development and application of an ab initio electronic structure method based on density functional theory, the orthogonalized linear combination of atomic orbital (OLCAO) method. The OLCAO method was initially developed at UW-Madison in mid-70s. Over the years, the method has been steadily improved, refined and withstood the test of time, and emerged as an extremely effective computational tool for complex materials. I will present three examples of its recent applications: (1) Densification of a near-perfect continuous random network model of amorphous SiO2 glass (Fig.1); (2) Genomic approach for the mechanical properties and electronic structure in a novel class of layered ternary compounds, the MAX phases (Mn+1AX2) (M = a transition metal, A= mostly Al or other group III, IV, V elements, X = C or N) (Fig.2); (3) Application to biomolecular systems and large proteins such as brome mosaic virus (1js9) (Fig.3). These examples illustrate the versatility of the OLCAO method in addressing specific problems of different material systems in diversified scientific and engineering fields. Further applications and limitations of the method will also be discussed.

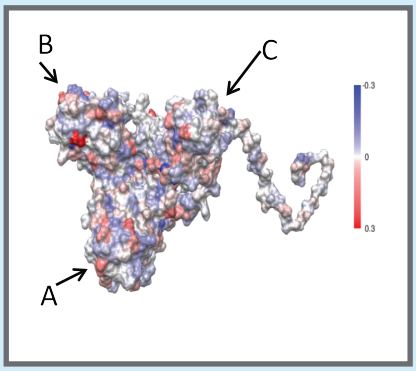

Figure 2

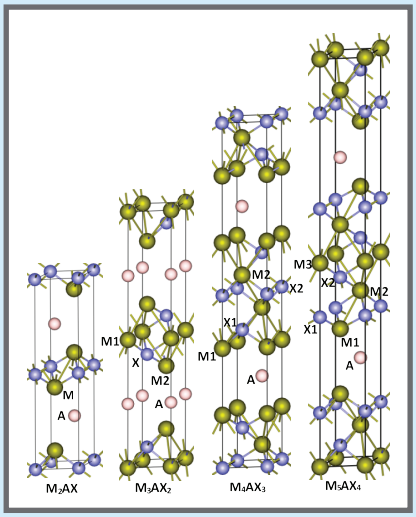

Figure 3

Thursday, March 27, 2014

3:30 pm | 5280 Chamberlin Hall

Refreshments will be served after the lecture at the Van Vleck Physics Faculty Lounge