



BILKENT UNIVERSITY

unam - INSTITUTE of MATERIALS SCIENCE & NANOTECHNOLOGY

FACULTY OF SCIENCE

**MATERIALS SCIENCE and NANOTECHNOLOGY
GRADUATE PROGRAM SEMINAR**

“Electronic structure calculations of nano solar cells”

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When constructed for device applications, a nanostructure rarely works alone. Free standing colloidal quantum dots/wires are often connected or blended with organic/biological molecules to provide structural supports and composite electronic, optical properties. Understanding the electronic structures and carrier transports of such mixed systems is often at the heart of nanoscience applications. For example, the inorganic-organic nanosystems can be used for photovoltaic solar cells and photochemistry fuel productions. Understanding and predicting the interface properties of these structures are critical to these applications. Theoretical simulation plays a pivotal role in studying these processes which are often poorly understood. Here, I will give a few examples of different nanostructures, which have potential applications for the electronic devices and solar cells. However, besides a few very expensive direct ab initio methods, currently there is a lack of practical methods to calculate and quantitatively predict the electronic properties of systems, which often contain a few thousands of atoms. Here, we propose to use the Linear Scaling 3 dimensional fragment (LS3DF) method for large scale nanomaterial simulations. The main idea of this approach is divide-and-conquer, and heart of this method is the novel patching scheme that effectively cancels out the artificial boundary effect, which exist in all divide-and-conquer schemes. This method has made ab initio simulations of the thousands-atom nano systems tractable in terms of simulation time, while pertaining essentially the same accuracy as the direct calculation methods. The LS3DF method has won the Gordon Bell Prize in SC 2008 for its algorithmic achievement. We have applied this method to study the electronic structures and the internal electrical field in the ZnO nanowires, which is also used for solar cells.

Date : August 6, 2010 (Friday)

Time : 15:40

Place : Faculty of Science Building, A Block, Seminar Room (SA 240)

Tea will be served after the seminar