



BILKENT UNIVERSITY

unam - INSTITUTE of MATERIALS SCIENCE & NANOTECHNOLOGY

FACULTY OF SCIENCE

**MATERIALS SCIENCE and NANOTECHNOLOGY
GRADUATE PROGRAM SEMINAR**

“Time Dependent Density Functional Tool of Quantum Espresso.
Application to visible range spectroscopy of sizeable systems and obtaining
insights regarding molecular excited states”

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TDDFPT is an implementation of the Lanczos-Liouville approach to linearized time-dependent density-functional theory. It is designed to be able to simulate the spectral properties of molecular systems made of up to several hundreds atoms in the optical range.

TDDFPT is open-source software distributed under the terms of the GPL as a component of QUANTUM ESPRESSO. As with other components, TDDFPT is optimized to run on a variety of different platforms, from laptops to massively parallel architectures, using native mathematical libraries and a hierarchy of parallelization layers.

Date : June 14, 2010 (Monday)

Time : 15:40

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