

MAR07-2006-005110

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

The European Theoretical Spectroscopy Facility

REX GODBY, University of York, U.K., and European Theoretical Spectroscopy Facility

The ETSF (www.etsf.eu) is being created as a permanent output of the EU-funded *Nanoquanta* Network of Excellence (www.nanoquanta.eu, 2004-8), which joins 10 groups and over 100 researchers in research on the theory and simulation of spectroscopy of electrons in matter, and related excited-state electronic properties including quantum transport. The ETSF is intended to contribute significantly to nanoscience and nanotechnology through the development and application of theoretical spectroscopy, involving close collaboration between theorists (the existing *Nanoquanta* groups together with further theoretical groups) and a new community of experimental and industrial researchers who wish to apply modern theories of spectroscopy. In this talk I shall review some of the scientific output of the project so far, including the development of new ideas and techniques in many-body perturbation theory and time-dependent density-functional theory, and their application to a variety of prototype and actual systems including quantum transport in nanostructures, optical absorption in biological molecules and advanced materials, optical properties of nanoclusters and nanotubes, non-linear optical response, and spectroscopies of complex surfaces. I shall also briefly describe the network's integration activities, including code interoperability and modularity, training of internal and external researchers, and the legal, financial and organizational preparations for the ETSF.