



FINAL REPORT

PUBLISHABLE SUMMARY

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Name, title and organisation of the scientific representative of the project's coordinator:

Professor Rex Godby, Professor of Theoretical Physics, University of York



Project website address: <http://ei3.etsf.eu/>

Section 0

Executive Summary

The ETSF e-Infrastructure project (full name “European Theoretical Spectroscopy Facility Integrated Infrastructure Initiative”) was a 3.5-year project that commenced in January 2008. The overall aim of the project was to allow the European Theoretical Spectroscopy Facility – established by the 10 European groups of the *Nanoquanta* Network of Excellence in the Sixth Framework Programme – to bring its capabilities to experimental and industrial users through cutting edge applications of ETSF codes and theories, to develop and prove new capabilities for future user projects by developing new codes and theories, and to make further improvements to the computational infrastructure of the ETSF, in partnership with the Barcelona Supercomputing Centre.

The European Theoretical Spectroscopy Facility (<http://www.etsf.eu>) consists of a core of 10 European Nodes, comprising 31 senior researchers and their groups (over 150 scientists in total), together with seven Associate Nodes which offer their complementary expertise to ETSF users while not participating in the management of the ETSF. The ETSF engages with users through biannual calls for proposals, creating a new concept of a “theoretical facility”.

By the end of the project (30 June 2011), substantial achievements have been made in all work packages, fully or largely achieving, and in many cases exceeding, all project objectives. 68 new user project proposals have been accepted from users and funded wholly or partly by the present project (with a further 41 accepted and funded from ETSF nodes’ own resources), to be carried out by ETSF scientists. Of these projects, 96 are collaborative project carried out by ETSF scientists on behalf of the user, and 13 are training projects which allow ETSF users to become expert in using our (freely available) simulation software themselves.

Our seven “beamlines” (i.e. our software and underlying theoretical developments that provide the ETSF with the capability to undertake user projects) have been maintained at the international leading edge through intensive research, allowing the ETSF to respond to the changing demands of users as the experimental facilities that they use become more sophisticated, and the systems that they study become more complex. In total, ETSF scientists published 441 papers in the international peer-reviewed scientific literature during the project, including 46 Physical Review Letters and 14 Applied Physics Letters. 31% of the publications were joint between two or more ETSF nodes, demonstrating the ETSF as an integrated facility as established in the earlier Nanoquanta Network of Excellence. Extensive structures for disseminating and communicating the ETSF’s activities, software and services have been established, and training in theory as well as the use of ETSF software is provided through several different channels.

These developments deliver the best possible service to present and future users of the facility, with the world-class ETSF scientific capabilities continuing to increase to address the needs of an expanding community of users.

Project web site: <http://ei3.etsf.eu>

Appendix D

References

This list shows all ETSF-I3 papers published in or submitted to the scientific literature during the project; not all are cited in the report. Publications labelled “(ETSF*)” are joint publications (more than one ETSF node), those labelled “(ETSF)” involve a single ETSF node.

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