Proceedings of the First International Workshop on the Theoretical Calculation of ELNES and XANES (TEX2008) (Nagoya, Japan, 2–4 July 2008)

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PREFACE

Proceedings of the First International Workshop on the Theoretical Calculation of ELNES and XANES (TEX2008) (Nagoya, Japan, 2–4 July 2008)

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Both electron energy loss near edge structure (ELNES) spectroscopy and x-ray absorption near edge structure (XANES) spectroscopy provide information on the local structural and chemical environments of selected elements of interest. Recent technological progress in scanning transmission electron microscopy has enabled ELNES measurements with atomic column spatial resolution. Very dilute concentrations (nanograms per milliliter or ppb level) of dopants can be observed using third-generation synchrotron facilities when x-ray fluorescence is measured with highly efficient detectors. With such technical developments, ELNES and XANES have become established as essential tools in a large number of fields of natural science, including condensed matter physics, chemistry, mineralogy and materials science.

In addition to these developments in experimental methodology, notable progress in reproducing spectra using theoretical methods has recently been made. Using first-principles methods, one can analyze and interpret spectra without reference to experiment. This is quite important since we are often interested in the analysis of exotic materials or specific atoms located at lattice discontinuities such as surfaces and interfaces, where appropriate experimental data are difficult to obtain. Using the structures predicted by reliable first-principles calculations, one can calculate theoretical ELNES and XANES spectra without too much difficulty even in such cases.

Despite the fact that ELNES and XANES probe the same phenomenon—essentially the electric dipole transition from a core orbital to an unoccupied band—there have not been many opportunities for researchers in the two areas to meet and discuss. Theoretical calculations of ELNES spectra have been mainly confined to the electron microscopy community. On the other hand, the theory of XANES has been developed principally by researchers in the x-ray community. Publications describing the methods have been written more-or-less independently by the two communities.

The three-day workshop on the Theoretical Calculation of ELNES and XANES (TEX2008) was planned to help remedy this situation. It aimed to demonstrate capability of state-of-the-art theoretical techniques to explain and predict ELNES and XANES spectra, and to allow deep discussion between scientists in the two communities. It also provided an excellent opportunity to introduce experimentalists to the computational techniques available. Invited talks and poster presentations by leading scientists were given on the first day, which was followed by tutorial sessions for five computer programs on the second and third days. Excellent lectures were given by Peter Blaha (Vienna, Austria) on the `WIEN2k` code, Chris J Pickard (St Andrews, UK) on the `CASTEP` code, John J Rehr (Seattle, USA) on the `FEFF8` code, Frank de Groot (Utrecht, The Netherlands) on the `CTM4XAS` code, and Hidekazu Ikeno (Kyoto, Japan) on the

first-principles CI-multiplet code. Thanks to the enthusiastic participation of more than 100 scientists from around the world, the workshop was a complete success. The aim of this special issue in *Journal of Physics: Condensed Matter* is to share with the readers the most up-to-date knowledge presented at the workshop. We believe this will prove useful as a reference for researchers in many different fields, as well as an overview of the current status and future directions of theoretical calculations for ELNES and XANES.

TEX2008 was a satellite meeting of the First International Symposium on Advanced Microscopy and Theoretical Calculations (AMTC1) (Nagoya, Japan, 29–30 June 2008), which was held in commemoration of the establishment of the Nanostuctures Research Laboratory (NSRL) at the Japan Fine Ceramics Center (JFCC) and as a daughter event of EXPO 2005, Aichi, Japan. A Grant-in-Aid for Scientific Research on Priority Areas 'Nano Materials Science for Atomic-Scale Modification' from the Ministry of Education, Culture, Sports and Technology (MEXT) and support from the Chubu Economic Federation for the workshop are gratefully acknowledged.