Theory and Computation for Synchrotron Radiation Experiments

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INTRODUCTION

This project provides "theory of the experiment", to enable the interpretation of experimental data gathered at synchrotron radiation facilities like the ALS. The focus is on modeling experimental techniques that require computational simulation in order to extract useful information such as atomic positions, distances and identities, as well as electronic and magnetic structures at surfaces and interfaces. Typical applications include photoelectron diffraction (PD) and x-ray absorption fine structure (XAFS). We welcome suggestions to help select future topics for theoretical and computational development.

COMPUTER CODES - PRESENTLY AVAILABLE

Three synchrotron-related computer codes are (as of Feb. 1999) available for free downloading from the web at http://electron.lbl.gov/software/:

- the MSCD package: to simulate core-level photoelectron diffraction for linear polarized light, including automated fitting of atomic coordinates to experimental data [1];

- REPS: to calculate core-level relaxation energies in photoelectron spectroscopy (using the equivalent-core approximation) [2];

- a holographic package: to reconstruct atomic structures from photoelectron and x-ray diffraction data (holograms) [3].

Further details about these packages can be found at the above mentioned web site.

In addition, the FEFF codes for XAFS are available from the FEFF web site at the University of Washington, Seattle, after obtaining a license [4].

COMPUTER CODES - IN PREPARATION

In collaboration with J.J. Rehr, the FEFF codes for XAFS [4] simulations will be installed to allow ALS users to run FEFF on ALS computers.

An expansion of the photoelectron diffraction package will introduce relativistic and magnetic spin effects, as well as circular and linear dichroism [5]. This will extend accurate studies to spin-dependent and light-polarization-dependent photoelectron diffraction.

A code to calculate valence-level photoelectron diffraction is under development [6]. It will permit the detailed study of the spatial distribution and energetics of valence electron levels at surfaces and shallow interfaces.

FURTHER INTERACTIONS

A Seamless Computing Environment is planned to integrate experiment, computation and theory at the ALS and elsewhere. Its goals include: unifying data formats; providing data analysis; interfacing with graphics and simulation; and enabling remote on-line collaborations with an electronic notebook.

Workshops with topical and tutorial emphases are planned to foster close interactions between experiment, computation and theory.

A Synchrotron Radiation Research Theory Network (SRRTNet) is being set up to interconnect related efforts world-wide: see http://electron.lbl.gov/srrtnet/srrtnet.html for the latest information.

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