# A comparison of low-Z EXAFS experiment and ab initio calculations

# A comparison of low-$Z$ EXAFS experiment and *ab initio* calculations

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**Abstract.** We report high-quality experimental fluorescence-yield EXAFS data and two different types of *ab initio* simulation (performed with MUFPOT, ICXANES, and FEFF) for O K-edge XAFS of NiO and $Cu_2O$. The results are indicative of the present 'state of the art' of EXAFS simulations for low-$Z$ atoms, including the effects of multiple scattering by the photoelectron. Employing the XAFS simulations to perform a quantitative analysis, the degree of accuracy for the determination of structural parameters, e.g. nearest-neighbour distance, is assessed. It can be agreed that with algorithms now available the problem for standard applications of the treatment of multiple scattering of a photoelectron above the threshold in the commonly used muffin-tin model potential has been solved. This granted, the remaining discrepancies between experiment and calculation disclose the relative significance of refinements to the model other than for the scattering, e.g. Debye–Waller factors, multi-electron effects or corrections to the potential.

## 1. Introduction

With the improving quality of experimental extended x-ray absorption fine structure (EXAFS) data more and more information can be extracted from the spectra. In the early days of EXAFS the main objective was to obtain the distance between the absorbing atom and the nearest neighbour [1]. However now longer distances or bond angles can be determined by taking into consideration multiple-scattering (MS) pathways for the analysis of the spectra [2, 3]. To obtain the full information contained in the EXAFS indirect methods have to be employed. Consequently the standards for the exactness of calculations have risen accordingly [4, 5]. In this context x-ray absorption spectra from low-$Z$ elements are particularly interesting. Taking into account the fact that these elements are usually surrounded by heavier atoms with large scattering amplitudes, simple geometrical considerations indicate that MS contributions should be significant in these spectra. So, not only do these spectra contain interesting structural information, they also can serve as a benchmark for current x-ray absorption fine structure (XAFS) simulation codes.

   In the following we report high-quality fluorescence yield (FY) O EXAFS spectra of NiO and $Cu_2O$ together with *ab initio* calculations of the EXAFS of these systems. The choice of NiO and $Cu_2O$ for our exemplary comparison of experiment and theory for low-$Z$ elements is explained by the different role of MS contributions in the fine structure of these systems, expected to be strong in NiO, because of favourable symmetry, and weak in $Cu_2O$. For thermal damping and expansion to be minimal we used spectra at low temperatures (30 K and 80 K) only.

   For the calculations the ICXANES code, developed by Durham *et al* [6] and updated by Vvedensky *et al* [7], applied here to the far edge region, was used. These are band-structure-type or cluster calculations that do include within a given cluster of atoms full

MS contributions. We therefore take them to be the standard for the accuracy that can be achieved within the MS formalism for the calculation of the XAFS. We also discuss calculations with the MS code FEFF (version 5.04), developed by Rehr *et al* [5, 8], based on the scattering path formalism, complementary to the ICXANES approach. Both are *ab initio* calculations with virtually no fitting parameters. This must be kept in mind when assessing the accuracy of the results.

## 2. Experimental details

The O K$\alpha$ FY EXAFS spectra of single-crystalline NiO and $Cu_2O$ were recorded at the storage ring BESSY with a windowless Si(Li) detector in ultra-high vacuum [9]. The use of FY detection for the examined systems has several advantages [9] compared to electron detection methods—a high signal-to-background ratio; a low surface sensitivity and large information depth providing high bulk sensitivity, charging of the sample causes no problems—all of which help to minimize possible errors while extracting the true EXAFS signal from raw data, and thereby warrant the good quality of the shown data. The energy resolution of the spectra is limited to 1–2 eV by the monochromator.

The samples were cooled down to 80 K for NiO and 30 K for $Cu_2O$, so that Debye–Waller damping of the signal is small and complications from anharmonicity effects are minimal [10, 11]. Further details of the experiment and the investigation of thermal damping and expansion in oxides and fluorides will be given elsewhere [12]. A good thermal contact was achieved by using a thin layer of In as an intermediate between sample and holder to which the samples were pressed close mechanically. The EXAFS was obtained from the FY data according to the procedure given by Tröger *et al* [13], clearing the raw spectra from self-absorption effects.

## 3. Applied numerics

The basic theory for XAFS [14] can easily be formulated in the picture of the muffin-tin model for the final-state potential. The absorption cross section then is given mainly by the inverse of a block matrix, containing the inverse atomic scattering matrices $(t^i)^{-1}$ as diagonal elements and the propagators between the atoms $g^{ij}$ as off-diagonal elements [15]. In terms of the physics involved this matrix inversion amounts to calculating the effective reflectivity of the cluster of atoms surrounding the central absorbing atom. Both $(t^i)^{-1}$ and $g^{ij}$ are given by their $(l, m)$ components in the partial wave expansion. The number of angular momentum components that have to be computed for this expansion to converge is growing with increasing energy. So the dimension of the matrix to be inverted is increasing accordingly (quadratically in $(l, m)$). This rapidly growing computational effort for the calculation of the absorption cross section explains why this exact method of matrix inversion is commonly applied only in the near edge region [16]. Nevertheless, in a little 'tour de force' of computing power, we continued calculations into the far-edge range of energies of 400–500 eV above the photoabsorption threshold.

In ICXANES the cluster consists of the central absorbing atom and the local environment out to a radial distance determined by the elastic scattering length of the emitted photoelectron. It is divided into concentric shells of atoms partitioning the one matrix for the whole cluster into a set of smaller matrices, one for each shell [17]. This approach of solving the MS equations first within each shell and then recursively between

the shells themselves and the central atom leads to a tractable cluster size of up to 150 atoms. Furthermore symmetry considerations are employed, identifying atoms identical under symmetry transformations and thereby reducing further the dimension of the matrices to be inverted. In our calculations, we used a maximum angular momentum for the atomic phase shifts of $L_{MAX} = 7$ and a maximum angular momentum for the symmetrized single-centre expansion of $L_{OUT} = 15$, as these quantities are defined in [17]. In order to obtain well converged results for high energies, because of increasing virtual memory and CPU requirements of the code we approached the limit of what is practicable for routine simulations of experiments on an ordinary workstation (Digital DecStation 5000/120). To give some idea, a simulation of a complete EXAFS spectrum for the highly symmetrical system of NiO took about six hours CPU time, a simulation of a spectrum for the more open structure of $Cu_2O$ already took about 100 hours CPU time.

For a calculation with ICXANES there are two physical parameters (as opposed to technical parameters for keeping the numerical expense to a minimum) to be set [7]: the cluster size, determined by the number of shells included, and the imaginary part $V_{Im}$ of the photoelectron energy as an empirical value to represent the decay rate of the excited state, being related to the photoelectron's mean free path $\lambda$ by

$$\lambda = \hbar^2 k / (m V_{Im}).$$

The wavenumber $k$ is defined by

$$k = (2mE)^{1/2} / \hbar$$

where $E$ is the kinetic energy of the photoelectron, i.e. the electron excited from a core state of energy $E_c$ by absorption of energy $\hbar\omega$ has an energy

$$E = E_c + \hbar\omega.$$

Contrary to common practice in near edge x-ray absorption fine structure (NEXAFS or XANES) and low energy electron diffraction (LEED) where this $V_{Im}$ is set to a constant value between 1 eV and 8 eV, here, because of the large energy range under investigation, this imaginary part of the energy is varied so as to model a $\lambda$ following the 'universal' curve [18].

The number of shells to be included has to be checked for each system. Figure 1 illustrates for the case of NiO how convergence is found using a cluster of seven shells, e.g. a cluster of 93 atoms with a maximum radius of 5.91 Å. The curves show calculations for clusters of increasing size, the first (bottom) one consisting of three shells only, the last (top) one of eight. Examining the fine structure we observe for a cluster size of less than six shells that adding one more shell of atoms to the cluster changes features of the spectrum, e.g. near $k = 3.4$ Å$^{-1}$ and $k = 7.2$ Å$^{-1}$. But obviously atoms further from the central absorbing atom than the seventh shell do no longer contribute significantly to the EXAFS of the system. For $Cu_2O$ eight shells had to be used, that is 95 atoms and a cluster radius of 6.29 Å.

As ICXANES only solves the scattering problem for a given configuration of partial-wave scatterers, the atomic partial-wave scattering-phase shifts for each atom type in the system have to be obtained from elsewhere. We used the Daresbury code MUFPOT [19]. We obtained best results by the use of the so-called 'relaxed and screened' potential [20] with atomic radii scaled until muffin-tin spheres touch. The potential is calculated according to the Mattheis prescription [21] with a constant real exchange correlation part in the potential. However this ground-state theory is somewhat inadequate for the description of the excited
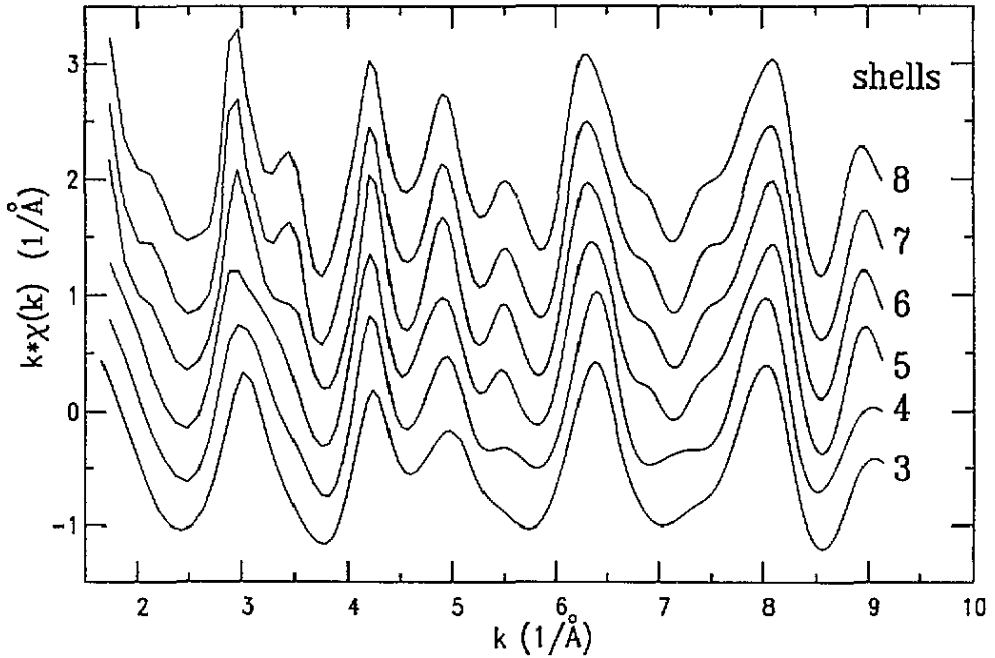
**Figure 1.** MS ICXANES calculations for NiO. Illustration of convergence of results with increasing cluster size. In the graph an arbitrary offset has been added to the curves.

state in the EXAFS experiment and a complex energy-dependent self-energy should be used instead [22] describing more correctly the quasiparticle decay by plasmon creation and the growing inefficiency of the electron gas in shielding a rapidly moving perturbation [23]. The chief error resulting from a ground-state theory results from the use of a constant muffin-tin zero, e.g. the energy zero of the photoelectron wavenumber. Therefore redefining the energy scale according to

$$E \rightarrow E' = E + \Delta(E)$$

with

$$\Delta(E) = \mathrm{Re}\,\Sigma(E) - V_{\mathrm{MT}}$$

corrects this [22]. Here $V_{\mathrm{MT}}$ is the constant muffin-tin value assumed by MUFPOT and $\Sigma(E)$ is the self-energy contribution to the muffin-tin potential in an excited-state theory for the photoelectron, replacing the constant exchange correlation potential. In the upper part of figure 2 the effect of this rescaling of the energy on the EXAFS spectra of $Cu_2O$ is illustrated, and in the lower part the constant muffin-tin zero energy $V_{\mathrm{MT}}$ and the energy-dependent real part of the self-energy $\mathrm{Re}\,\Sigma$ are shown. It should be noted that only for high $k$ values is this scaling asymptotically linear and it will influence the Fourier spectrum of the data. We obtained $\mathrm{Re}\,\Sigma(E)$ from the program code FEFF, which uses the Hedin–Lundqvist self-energy.

The FEFF code comprises all of the calculation in one package [5], the calculation of the model potential from atomic charge densities, the determination of the atomic partial-wave scattering-phase shifts, and the solution of the scattering problem for the excited final state
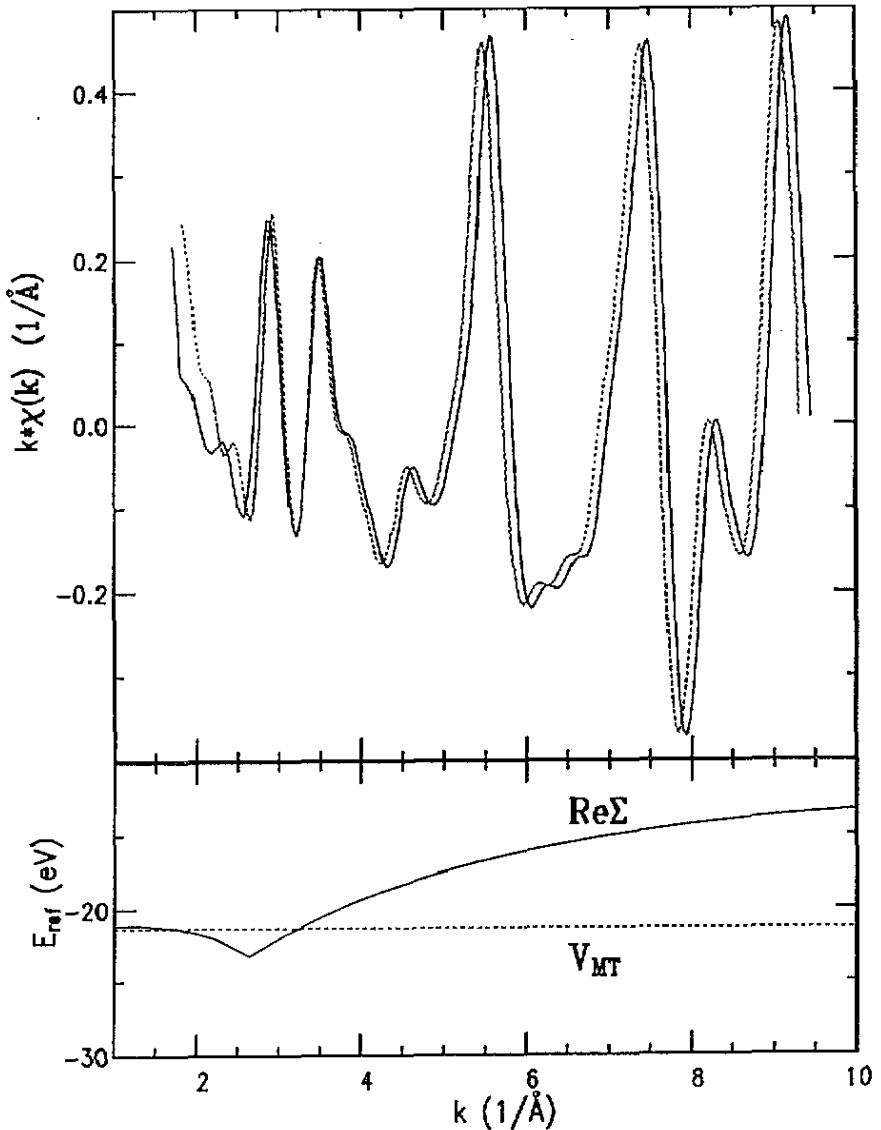
**Figure 2.** Energy-reference correction to ground-state theory: upper part, MS ICXANES calculations for $Cu_2O$ with constant muffin-tin zero (broken curve) and energy-rescaled (full curve) as explained in the text; lower part, illustration of difference between constant and energy-dependent energy references.

to obtain the absorption coefficient. The differences from a calculation by MUFPOT and ICXANES are: (i) for the calculation of the potential the excited-state self-energy is used instead of a ground state exchange-correlation potential, and consequently complex partial-wave phase shifts and a defined energy reference for the photoelectron are obtained; and (ii) for the scattering problem the scattering-path approach [8] is used. In other words the matrix inversion of the problem is expanded into a series in orders of scattering events at different atomic scattering sites that is programmed very efficiently using a separable representation of the electron propagators [24] and carried out until some criterion of convergence is

satisfied, the maximum value of angular momentum used in our FEFF calculations being $l$ = 24. Consequently the complex scattering process can be disentangled to its contributions from individual scattering paths. To a certain degree this is achieved in ICXANES, too, discriminating between inter- and intrashell scattering and allowing for a controlled number of intershell MS events, if desired [7]. This then also provides the option for single scattering only with the result being equivalent to a curved-wave single-scattering [25] calculation. Due to the effective MS path approach used in FEFF, the time required for both our $Cu_2O$ and NiO calculations was about 15 min CPU time (on a DecStation 5000/120).

## 4. Results and discussion

The structural data used for the calculations have been taken from standard x-ray diffraction data tables [26]. NiO has a sodium chloride structure [27] with octahedral coordination of each atom and a lattice constant $a_0 = 4.172$ Å (at $T = 80$ K) whereas $Cu_2O$ has a $T_h^2$ cubic structure with two molecules in the unit cube ($a_0 = 4.265$ Å at 30 K) where each Cu atom has two close O neighbours and each O atom is surrounded by four Cu atoms.
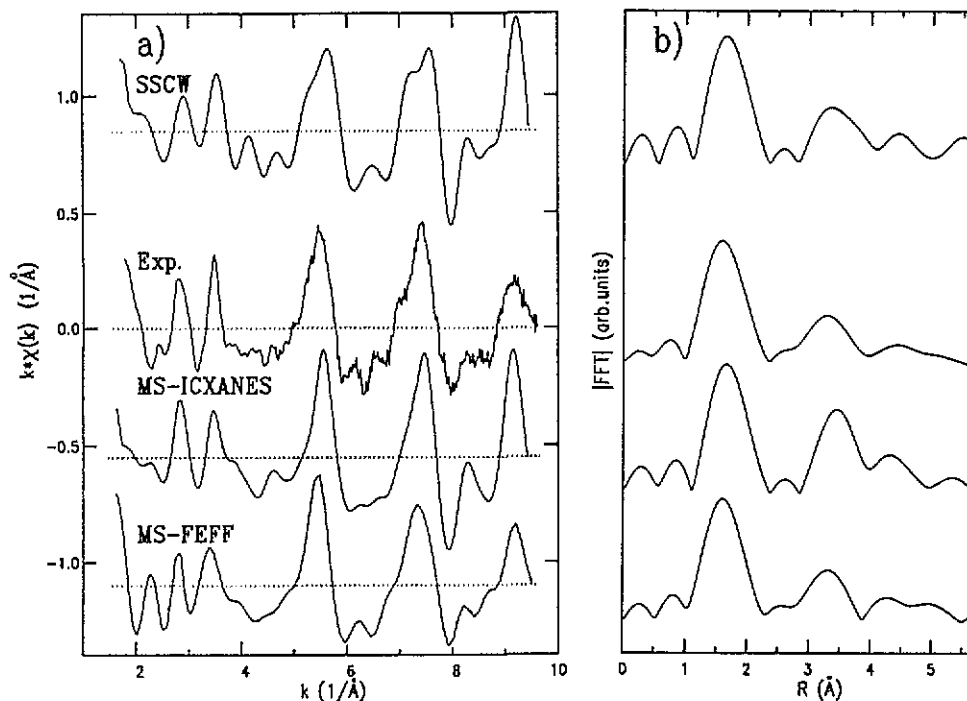


**Figure 3.** (a) O K-edge XAFS spectra for $Cu_2O$. From top to bottom: SSCW calculation, FY experiment (30 K), MS ICXANES calculation, MS FEFF calculation. An arbitrary offset has been added to the curves; the zero is indicated by a horizontal line. (b) Corresponding Fourier spectra.

In figure 3 we show our results for $Cu_2O$. Figure 3(a) contains the XAFS $k\chi(k)$, figure 3(b) the square moduli of the Fourier transforms of the spectra. The transformed $k$ range of the spectra is $k = 3.7$–$9.3$ Å$^{-1}$. In the experiment the inflection point of the O K-edge was used as the energy reference $E_0$. For comparison the calculations had to be shifted

with respect to the experiment by $\Delta E_0 = +6$ eV for ICXANES results and $\Delta E_0 = -7$ eV for FEFF results. All calculations with scattering-phase shifts input from MUFPOT, i.e. the single-scattering and the multiple-scattering ICXANES calculations, are energy rescaled as described in section 3. An amplitude reduction factor $S_0^2 = 0.5$ was used for ICXANES, matching amplitudes of experiment and calculation at $k \simeq 5$ Å$^{-1}$. This large $S_0^2$ is due to the fact that there is no thermal damping of the signal contained in our calculation [28] and losses due to multi-electron excitations, i.e. plasmons, are approximated only by an empirical $\lambda$ [7]. In FEFF calculations Debye–Waller factors for the atoms in each shell are employed using a correlated Debye model [30, 8] with Debye temperature and temperature of the set-up as input parameters. Taking a Debye temperature of $\theta = 400$ K an amplitude reduction factor $S_0^2 = 0.7$ was used to match the experiment, lying at the lower end of the expected range of values [31]. At this point it should be mentioned that the correlated Debye model is appropriate only for homogeneous systems. Therefore a deviation of our choice for $\theta$ from calorimetrically determined values need not be much of concern.

In figure 3(a) the top curve shows a converged single-scattering calculation, i.e. a cluster of eight shells, performed with ICXANES; the second curve is the experimental data. One frequency prevails in the spectrum which therefore can be expected to be well tractable with standard Fourier-transform techniques. Accordingly a well separable first peak in the Fourier spectrum is found. Nevertheless discrepancies between single-scattering calculation and experiment at remarkably high energies, i.e. between 6 Å$^{-1}$ and 7.5 Å$^{-1}$, can be seen. Furthermore the amplitude above $k = 8.5$ Å in the calculation is far too strong. The third curve shows a full-MS calculation performed with ICXANES, using the same input scattering-phase shifts and the same cluster of eight shells as for the single-scattering calculation, but setting no limit to the order of included inter- or intrashell scattering events. The experiment is remarkably well reproduced for the whole $k$ range observed; only the damping of the high-$k$ part remains too weak. Specifically, comparing the Fourier transforms of the above spectra, it can be deduced that the damping of the EXAFS contribution due to the second shell of Cu atoms is underestimated by ICXANES. This is caused by the actual $k$ dependence of the amplitude-reduction factor and the effect of atomic vibrations. Obviously more parameters are needed (i.e. Debye–Waller factors) in order to properly model the amplitudes of the higher-frequency contributions to the Fourier transform. As these are however the first EXAFS *ab initio* calculations using ICXANES we wanted to keep the number of fitting parameters to a minimum and Debye–Waller factors were not taken into consideration. Consequently in the MS FEFF calculation (figure 3(a) bottom curve), when Debye–Waller factors are employed, better agreement in the overall amplitudes is found. Here MS contributions up to fifth order, that is contributions from all scattering paths for the photoelectron with up to five scattering events, have been included. It can be seen that for the NEXAFS regime ($k \leqslant 4$ Å$^{-1}$) this is still not sufficient, but for short distances ($R \leqslant 5$ Å), e.g. the large frequencies in the EXAFS, Fourier transforms of experiment and FEFF correspond almost perfectly.

To assess the quantitative exactness of these calculations we performed a Fourier-fit analysis of the first-shell Fourier peak: the nearest-neighbour O–Cu contributions to the EXAFS, well separable in the Fourier spectra (see the first peaks in figure 3(b)), are Fourier back transformed, and then fitted in $k$ space. Using the different calculations as different standards yields the distances summarized in table 1 when the experiment is fitted to these standards, with the distance $r$ as a free parameter and $E_0$ fixed in agreement with figure 3(a). As reference in the first row of table 1 the x-ray diffraction value at 30 K is given. In the EXAFS experiment an *effective* pair distribution function is probed [32]. Therefore, e.g. for Cu$_2$O at low temperature, the distance determined from EXAFS is 0.003 Å smaller than the

**Table 1.** O–Cu nearest-neighbour distance $r$ in $Cu_2O$. Values are given as obtained from a Fourier-fit analysis. The calculations have been used as different standards for the distance determination.

| Source | $r$ (Å) |
| --- | --- |
| X-ray diffraction at 30 K | 1.846(3) |
| MS ICXANES (unscaled) | 1.831 |
| MS ICXANES (scaled) | 1.851 |
| Single-scattering ICXANES (scaled) | 1.859 |
| MS FEFF | 1.837 |
| Teo/Lee [4] | 1.800 |

physical distance [12]. The $r$ values obtained from simulations in table 1 are corrected using this value. We find that largest deviations from the x-ray diffraction value are obtained when no rescaling of the energy (see section 3) in ICXANES/MUFPOT calculations is performed. Obviously this is mainly due to the differences in treatment of the model potential for the photoelectron in MUFPOT, as ICXANES results improve greatly when energy rescaling is done. However, it appears that the rescaling algorithm used is not optimal since it slightly overcompensates for the self-energy correction. The scaled MS ICXANES result and the MS FEFF result agree equally well, within less than one hundredth of an Ångström, with the true value. In FEFF calculations errors of this order may be caused by an imperfect description of the imaginary part of the potential [33, 34]. In contrast to these results the single-scattering (SSCW) curved-wave calculation gives a distance more than 0.01 Å too large. Nevertheless all curved-wave calculations yield values considerably improved from a plane-wave treatment [4].

In Figure 4 the results for NiO are shown. For a comparison with the experiment the calculations again had to be shifted by $\Delta E = +7$ eV for ICXANES results and $\Delta E = -10$ eV for FEFF results. The experimental data for NiO have been collected at a different beamline from those for $Cu_2O$. Note the better statistics. To match the experiment $S_0^2 = 0.5$ was used for ICXANES calculations; for FEFF calculations a Debye temperature of $\theta = 620$ K and an amplitude reduction factor of $S_0^2 = 0.7$ were used. Examining the spectra the situation appears to be more complex than in figure 3, because of strong MS and correlation effects [35]. The fine structure cannot be divided into a NEXAFS and an EXAFS regime with interference of multiple-shell contributions in the NEXAFS domain only. Therefore single peaks in the Fourier transforms shown in figure 4(b), taken from a $k$ range of $k = 1.75$–$8.85$ Å$^{-1}$, *do not lend themselves to any quantitative structural analysis.* To give some idea, those intensities in the Fourier spectrum marked by the broken window in figure 4(b) contain single-scattering contributions from the first three shells plus MS contributions from three important triangle scattering paths (O–O–Ni–O, O–Ni–Ni–O, O–Ni–O–O), at least. We found that not only is none of the peaks clearly separable from the rest, but also the Fourier peak position is highly sensitive to the choice of the transformed $k$ range and that the quality of the reproduction of small features in the fine structure spectrum, e.g. the wiggle near 3.5 Å$^{-1}$, can shift the whole Fourier spectrum of the calculation with respect to that of experiment; all of which will inflict considerable ($\sim 0.05$ Å) errors on a standard Fourier analysis of the spectrum [34].

Nevertheless several facts can be learned from a direct comparison of the experimental and calculated XAFS themselves (figure 4(a). First, we remark again the dramatic improvement of the calculation when MS is included (compare the first and third curves from the top). Again these calculations use the same cluster of atoms (seven shells) and identical sets of scattering-phase shifts, and differ only in the inclusion of MS contributions
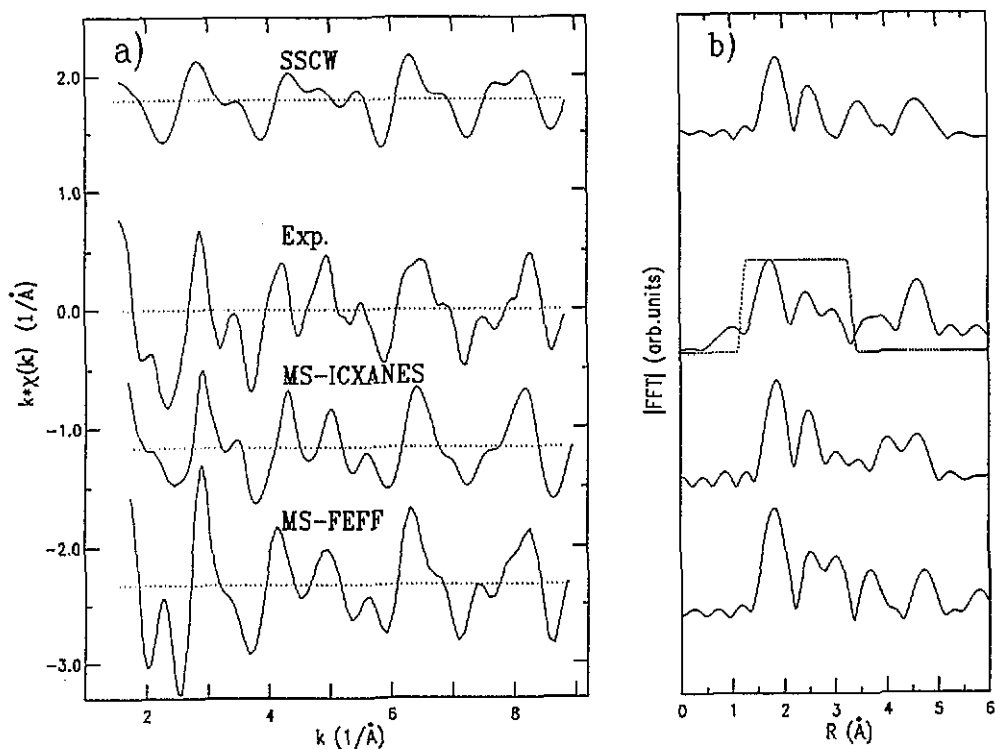
**Figure 4.** (a) O K-edge XAFS spectra for NiO. From top to bottom: SSCW calculation, FY experiment (80 K), MS ICXANES calculation, MS FEFF calculation. An arbitrary offset has been added to the curves, the zero is indicated by a horizontal line. (b) Corresponding Fourier spectra.

for the latter. Also subsequent energy rescaling has been performed with both of them. The MS ICXANES calculation reproduces virtually all experimental features, so we are confident that the MS of the photoelectron has been treated correctly, although some amplitude relations are wrong and some features seem to be overdamped. Strikingly the FEFF result (bottom curve), which includes MS contributions up to sixth order, shows similar discrepancies in the amplitude relations. Compared to the completely temperature-independent ICXANES calculation the correlated Debye model employed in FEFF to simulate vibrational losses of the photoelectron in the crystal does not seem to be of much advantage. In general the inadequacy of the treatment of vibrational effects seems to be one of the limiting factors for the accuracy of the simulations, bearing greater significance with increasing complexity of the investigated system.

Both types of *ab initio* code show a good correspondence to experiment. Detailed inspection of the data suggests that FEFF agrees slightly better at high energies and ICXANES at low energies. The quality of reproduction is excellent bearing in mind the *ab initio* nature of the simulations. The FEFF calculation within the scattering-path formalism seems to converge very well towards the full-MS band-structure type calculation of ICXANES. This convergence is weakest in the near-edge region and the cut-off criterion for the inclusion of paths in the MS expansion of FEFF should probably be extended here. On the other hand, it is the very power of scattering-path formalism to yield excellent results with reasonable speed [24] by including only the most important scattering paths. This code will slow down, too, when the limit of including all paths is approached.

In spite of the energy rescaling performed with the results, there remains a small scaling effect between ICXANES/MUFPOT calculations and experiment on the one hand and FEFF on the other, indicating that the insufficient treatment of the self-energy in MUFPOT cannot be remedied completely this way.

Furthermore two details in the experimental EXAFS remain unaccounted for by a single-electron MS theory. Neither the small nose near 5.3 $\text{Å}^{-1}$ nor the double peak character of the maximum near 6.4 $\text{Å}^{-1}$ in figure 4(a) have been found in any of the calculations we performed, although both features also appear in total electron yield measurements, see for example [36]. These features might be due to multielectron effects, as they have been reported in EXAFS spectra before [37].

## 5. Conclusion

We have shown by explicit comparison for $Cu_2O$ and NiO of experimental O FY EXAFS and theoretical calculations that light elements, too, can be investigated using simulation codes established to yield good results in the hard-x-ray domain. Applying two different codes with two different approaches to the scattering problem, i.e. band-structure-type calculation by ICXANES and scattering-path expansion by FEFF , and observing the correspondence of their results, we verify that a complete treatment of the scattering process is no longer a problem. In the light of applications where information can only be extracted by comparison of experiment and model calculations this is an important prerequisite. For $Cu_2O$ we illustrate that when Fourier methods can be applied these calculations yield nearest-neighbour distances correct to within 0.01 Å of the expected value. We did not come across any unexpected difficulties applying currently available XAFS theories to the soft-x-ray domain of low-$Z$ EXAFS. The observed convergence of results within the scattering-path formalism towards those of band-structure-type calculations is affirmative and confirms that for a great many systems theoretical standards are now easily available.

To establish the significance of these simulations we wish to point out that *ab initio* calculations such as those presented here provide the only test of structural models against sufficiently complex experimental data, e.g. strong MS, close shells, short accessible $k$ range, and it has proved useful to be able to compare the results from both types of calculation. These calculations are now accessible also for light elements, such as O, in bulk materials and on surfaces. Information for these complicated systems has to be extracted by comparison of experiment and calculation, similar to the standard NEXAFS or LEED procedure, with the whole crystal structure as a parameter set that has to be determined in an iterative process until optimal reproduction of the experiment is achieved. It can be imagined that quantitative measures, such as $R$ factors, will be introduced in future here, too.

Nevertheless we find that for systems that show strong MS and high correlation, such as NiO, it does not suffice to handle properly the scattering only. Multielectron and phonon excitations should be taken into account. With increasing complexity of the investigated system—i.e. more relevant atoms and MS—the use of a correlated Debye model to approximate the crystal's phonon density of states becomes more questionable, as the calculations for NiO showed. Refined models to embrace better lattice dynamics in the calculation of the EXAFS will have to be found to remove remaining discrepancies.

## Acknowledgments

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[27] The very small rhombohedral distortion in the antiferromagnetic phase of NiO is neglected here.
[28] In ICXANES a temperature dependence could be achieved employing temperature-dependent partial-wave scattering-phase shifts [29], but this would be equivalent only to an isotropic x-ray Debye–Waller factor and not take into account the correlation effects in the EXAFS Debye–Waller factor [30]. However it has been checked that ICXANES and FEFF results yield the same amplitudes when temperature dependence is neglected in both codes, i.e. an infinite Debye temperature for FEFF.
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