Electronic supplementary information of:

Multi-scale theoretical approach to X-ray absorption spectra in disordered systems: an application to the study of Zn(II) in water

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We provide as electronic supplementary information (ESI) the input files and all possible instructions to reproduce the results presented in the main article.

Molecular dynamics with dummy cations

Attached are the instructions for the topology construction that can be performed with the code psfgen (part of the NAMD distribution). The file is: top_dummies.rtf . This can be loaded by psfgen with the instructions included in: dummies.tcl . Parameters for these cations used in the molecular dynamics simulations are in the NAMD file: par_dummies.prm . These parameters have been attached to the TIP3P force-field for water molecules, the latter available in all molecular dynamics packages.

DFT calculations

Attached are the pseudopotential files, in the unified pseudopotential format (UPF), generated with the atomic LD1 code of the Quantum-ESPRESSO package and with DFT approximations used for the molecular systems (see main text for details). The LD1 code performs the calculation of electronic states of isolated atoms with: i) all electrons; ii) with a pseudopotential representing the core electron density and a set of complementary valence electrons; iii) comparing the two calculations. The input file for the atomic code LD1 are reproduced, for Zn, in the UPF file. The files for H and O provide the results for liquid water similar to those available in the Quantum-ESPRESSO web-site. The core wave-function required by XSpectra can be extracted from the last zinc pseudopotential file using the atomic tools of the package.
The files are:
hydrogen H.pbe-rrkjus.UPF ;
oxygen O.pbe-van.UPF ;
zinc Zn.pbe-spn-rrkjus.UPF ;
zinc with 1s electron extracted Zn.star1s-pbe-spn-rrkjus.UPF .

One of the input files for the relaxation steps, performed with the PW code of Quantum-ESPRESSO, is provided in: relax.in .

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The relaxed configuration is finally used as the input coordinates for the calculation of the electron ground state in the presence of the hole in the 1s state of zinc core. This is performed with the input file scf.in .

The dielectric environment of bulk liquid water is described in the input file required by the code Environ of Quantum-ESPRESSO: environ.in .

Calculation of XANES spectra

The input file for the XSpectra code is in: xspectra.in .

The calculation must be performed with the three direction of polarization (the cartesian axes in the vector xepsilon) and the three resulting spectra are averaged in space.