# Validation of *ab initio* molecular dynamics simulations of ZnO using the Zn K-edge EXAFS spectra

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Wurtzite-type zinc oxide (ZnO) is widely used material with pronounced structural anisotropy along the c-axis, caused by relative displacement of two interpenetrating hexagonal close-packed sublattices, each built up by one type of atom (Zn or O). The anisotropy of ZnO structure affects strongly its lattice dynamics and determines its piezoelectric and pyroelectric properties. It is also responsible for a slight distortion of $ZnO_4$ tetrahedra, which is temperature dependent. Such peculiarities of the ZnO structure and dynamics are a problem for their accurate description using classical force-field models [1], which are often employed in the simulations of ZnO nanostructures.

An alternative, although more computing intensive, way to address this problem is to use the ab initio molecular dynamics (AIMD) simulations. In this study, we performed temperature dependent AIMD calculations of wurtzite-type ZnO bulk phase and validated the obtained theoretical results by direct comparison with the experimental Zn K-edge extended X-ray absorption fine structure (EXAFS) spectra as suggested in [2]. The AIMD simulations were performed based on Kohn-Sham density functional theory (DFT) by the CP2K code at three temperatures (300, 600 and 900 K) using "Piz Daint" supercomputer at the Swiss National Supercomputing Centre.

Atomic configurations obtained from AIMD trajectories were used to follow a number of useful properties as, for example, ZnO lattice dynamics and an anharmonicity of the Zn-O bonds with special attention to correlation effects in atomic motion. Distributions of bond angles and thermal ellipsoids have been analysed. Mean-Square Relative Displacement (MSRD) values obtained in AIMD were compared with the MSRD values obtained using reverse Monte Carlo method from the analysis of EXAFS data [1].

The advantages and limitations of AIMD approach will be discussed.

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