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Density Functional Theory modeling of the structural and isotopic properties of ZnO surfaces

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ZnO are very common systems present in various contexts and also model systems widely studied. ZnO nanoparticles are found in soil and water, it is therefore important to study the fate and behavior of this material in the environment, and isotopes are efficient tools for achieving this goal. Computer simulations can complement the direct materials analysis of these systems. In particular, we focused our theoretical study on the assessment of the surface effect on the isotopic signature. Do ZnO nanoparticles have different Zn isotope composition from bulk ZnO crystals in equilibrium conditions? In order to address this question, we performed structure and frequency calculations based on density functional theory (DFT) on various structural models. Isotopic properties are then determined from the vibrational frequencies. Three kinds of structural models were considered: ZnO bulk structure, the slab surfaces (10-10) and (2-1-10), and a model nanoparticle. The results obtained allow us to discuss the surface effect and the isotopic properties of ZnO nanoparticles.