

Abstract Submitted
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Impact of the vapour pressure of water on the equilibrium shape of ZnO nanoparticles: An ab-initio study STEPHANE KENMOE, MIRA TODOROVA, P. ULRICH BIEDERMANN, JOERG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH — ZnO powders and nanoparticles are used as catalysts and have potential applications in gas-sensing and solar energy conversion. A fundamental understanding of the exposed crystal facets, their surface chemistry and stability as function of environmental conditions is essential for rational design and improvement of synthesis and properties. Using density-functional theory calculations we study the adsorption of water on the non-polar low-index $(10\bar{1}0)$ and $(11\bar{2}0)$ surfaces of ZnO. Observing both molecular and dissociative H_2O adsorption, we analyse the contributions of water-surface and water-water interactions to the energies of the stable structure. Based on this insight we compute and analyse the impact of water adsorption on surface energies and the equilibrium shape of nanoparticles in a humid environment.

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