

Abstract Submitted
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An ab-initio study on the stability of ZnO(0001)-Zn surfaces in an electrochemical environment SU-HYUN YOO, MIRA TODOROVA, JOERG NEUGEBAUER, Department of Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — Zinc oxide, a wide bandgap semiconductor, is widely studied due to its various applications in different fields such as (photo-)catalysis, protective coatings, optoelectronics and others. Understanding the impact an aqueous environment has on the ZnO properties is important for several of these. Focusing on the polar Zn terminated ZnO(0001) surface we combine density functional theory (DFT) calculations with thermodynamic concepts to study the stability of surface structures in contact with different environments. Extending our previous studies on the stability of ZnO(0001) surface phases in dry and humid environment [1], we utilize our recent developments [2] to construct surface Pourbaix diagrams, which describe surface stability in dependence of the pH and electrode potential conditions of the aqueous environment. We find that the presence of the solvent has a large qualitative effect on the phase diagram stabilising triangular structures over adatom/vacancy-type structures. [1] M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. 103, 065502 (2009) [2] M. Todorova and J. Neugebauer, Phys. Rev. Applied 1, 014001 (2014)

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