

Abstract Submitted  
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**Hydrogen Adsorption on polar ZnO(0001)-Zn - extending equilibrium surface phase diagrams to kinetically stabilised structures** MIRA TODOROVA, Dept. for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany, MARKUS VALTINER<sup>1</sup>, Dept. for Interface Chemistry and Surface Engineering, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany, JOERG NEUGEBAUER, Dept. for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — Hydrogen adsorption on the Zn-terminated polar ZnO(0001) surface is studied by a combination of density-functional theory calculations and *atomistic thermodynamics*. Going beyond the thermodynamic limit and constructing meta-stable phase diagrams we extend the concept of equilibrium surface phase diagrams to include kinetically stabilised surface reconstructions. Using this approach we were able to identify new and hitherto not reported structures that become stable under non-equilibrium extreme H-rich conditions. Experimental situations that realise such conditions will be discussed.

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