Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Adsorbate phases of H on ZnO $(10\bar{1}0)$ **surface as a function of temperature and pressure from first principles** MARIA E. STOURNARA, SERGEY V. LEVCHENKO, Fritz-Haber-Institut der MPG, Berlin, DE, SANTIAGO RIGAMONTI, MARIA TROPPENZ, Humboldt-Universität zu Berlin, Berlin, DE, OLIVER T. HOFMANN, Technische Universität Graz, Graz, AT, PATRICK RINKE, Aalto University, Helsinki, FI, CLAUDIA DRAXL, Humboldt-Universität zu Berlin, Berlin, DE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Zinc oxide (ZnO) is a highly multifunctional material with unique properties and a wide range of applications. To understand atomic hydrogen adsorption on the thermodynamically stable $(10\bar{1}0)$ surface at realistic H chemical potentials, we combine a first-principles cluster-expansion approach with *ab initio* atomistic thermodynamics. Our study reveals that at coverages below 6%, H atoms adsorb exclusively on surface O. At higher coverages, H adsorbs also on Zn, but there is an excess of O-H over Zn-H at all coverages, except 50% and 100%. Due to an interplay of long- and short-range electrostatic interactions, neighboring O-H/Zn-H pairs form chains along surface -O-Zn- rows, with each chain anchored at the excess O-H, in a wide range of (T, p_{H_2}). Our results offer a "road map" for H adsorption on the ZnO $(10\bar{1}0)$ surface at various conditions, consolidating findings from previous experiments [1-4]. —[1] Y. Wang *et al.*, PRL 95, (2005); [2] K. Ozawa and K. Mase, Phys. Stat. Sol. App. Mat. Sci. 207, (2010); [3] K. Ozawa and K. Mase, PRB 83, (2011); [4] J. Deinert *et al.*, PRB 91, (2015).

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Date submitted: 10 Nov 2016 Electronic form version 1.4