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Temperature stabilised surface reconstructions at polar ZnO(0001) MIRA TODOROVA, Department for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, MARKUS VALTINER, Christian Doppler Laboratory for Polymer/Metal Interfaces, Max-Planck-Insitut fuer Eisenforschung GmbH, Duesseldorf, GUIDO GRUNDMEIER, Christian Doppler Laboratory for Polymer/Metal Interfaces, MPI; Technical and Macromolecular Chemistry, University of Paderborn, Paderborn, JÖRG NEUGEBAUER, Department for Computational Materials Design, Max-Planck-Insitut fuer Eisenforschung GmbH, Duesseldorf — Combining diffraction experiments with density-functional theory calculations and thermodynamic considerations we study the atomic structure of the polar ZnO(0001) surfaces. We show that a large number of very different reconstructions with similar stoichiometry are energetically almost degenerate, thus surface vibrational entropy contributions significantly affect their stabilisation. The large impact of the vibrational entropy on the surface structure gives rise to a strong dependence of surface phase diagrams on temperature and enables us to consistently describe and explain the experimentally observed surface structures on polar ZnO(0001) surfaces.
M. Valtiner, M. Todorova, G. Grundmeier, and J. Neugebauer, Phys. Rev. Lett. 103, 065502 (2009).

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