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Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces DANIEL BERGER, Technische Universität München, Garching, DE, SERGEY V. LEVCHENKO, SASWATA BHATTACHARYA, Fritz-Haber-Institut der MPG, Berlin, DE, KARSTEN REUTER, Technische Universität München, Garching, DE, LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, Berlin, DE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE; Technische Universität München, Garching, DE — Introducing charge carriers into MgO via p doping greatly reduces formation energy of an O-vacancy in the bulk and at the (100) surface [1]. In this work, we use hybrid density functional theory to explore O-vacancy and O/O_2-ad-species defects at corners of MgO surfaces. The defects are modelled using MgO clusters embedded into a field of norm-conserving pseudopotentials and point charges. The long-range response of the oxide to the charge carriers trapped at the defects is taken into account using a polarizable force field. The low-energy defect atomic structures are found using an *ab initio* genetic algorithm [2]. Concentrations of O-vacancies and O-ad-species at realistic temperatures and pressures are obtained with *ab initio* atomistic thermodynamics. Unexpectedly, we find that O-ad-species rather than O-vacancies are dominating defects at realistic conditions. The stability of the O-ad-species over O-vacancies and pristine corners is explained by an interplay between bond-breaking, bond-making, and charge-carrier trapping. − [1] N. Richter *et al.*, Phys. Rev. Lett. **111**, 045502 (2013); [2] S. Bhattacharya *et al.*, New J. Phys., in press (2014)

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