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Charged and neutral oxygen vacancies at MgO surfaces under realistic temperature and pressure conditions NORINA A. RICHTER, SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Surface O vacancies (F-centers) can strongly influence catalytic properties of MgO and metal clusters supported on MgO, but the experimental determination of their concentration at catalytic conditions is difficult. We employ density-functional theory and the *ab initio* atomistic thermodynamics approach to determine concentration and charge states of F-centers at (111) and flat and stepped (100) surfaces of MgO at realistic (T, p) conditions. Slab models and the virtual-crystal approximation [1] are used to model charged defects at surfaces. We find a strong dependence of F^+ and F^{2+} formation energy on the exchange-correlation (XC) functional. Varying the amount of screening and fraction of exact exchange within the HSE functional, we find a linear correlation between defect formation energies and calculated valence-band width of the host material, in line with recent results for bulk systems [2]. Using this correlation and extrapolating to experimental band width, we conclude that only F^{2+} centers can be present in significant concentrations at the (100) terraces at realistic conditions. — [1] L. Vegard, Z. Phys. **5**, 17 (1921); M. Scheffler, Physica **146B**, 176 (1987); [2] R. Ramprasad *et al.*, subm. to Phys. Rev. Lett.

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