Abstract Submitted
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Concentration of point defects at metal-oxide surfaces: case study of MgO (100)[1] NORINA RICHTER, SERGEY LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany, SABRINA SICOLO, JOACHIM SAUER, Humboldt-Universitaet zu Berlin, Berlin 10099, Germany — We calculate from first principles the concentration of neutral and charged oxygen vacancies on a doped MgO (100) surface at realistic (T, p_{O_2}) conditions. Vacancy formation energies are computed using hybrid density-functional theory with parameters of the exchange-correlation functional adjusted according to a basic consistency requirement on the Kohn-Sham and G_0W_0 defect transition levels. The parameters are validated by CCSD(T) calculations of formation energies for neutral vacancies using embedded cluster models. Gibbs free energies of formation are obtained using the *ab initio* atomistic thermodynamics approach.[2] We demonstrate that the concentration of surface vacancies is significantly increased due to band bending and Fermi level pinning at the surface, resulting in lower formation energies of charged vacancies.

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[2]K. Reuter and M. Scheffler, Phys. Rev. B **65**, 035406 (2001); C. M. Weinert and M. Scheffler, Mat. Sci. Forum **10-12**, 25 (1986); M. Scheffler and J. Dabrowski, Phil. Mag. A **58**, 107 (1988)

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