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Formation of islands of substitutional Li defects on the MgO (001) surface SERGEY V. LEVCHENKO, MATTHIAS SCHEFFLER, Fritz Haber Institute of Max Planck Society — We use density functional theory (DFT) calculations to evaluate electronic structure and formation energies of the substitutional Li defects in the (001) surface, subsurface, and bulk MgO. We analyze the sensitivity of the results to the approximations in the exchange-correlation functional by comparing semi-local (GGA PBE) and non-local (PBE0 and B3LYP) approximations. Calculated formation energies indicate that the Li defects prefer to form islands with molar concentration 50% at the top layer, but not in the deeper layers. The formation energy of an isolated substitutional Li defect increases with the depth of the layer in which the defect is formed. We perform an *ab initio* atomistic thermodynamics [1] analysis to determine the average island size under realistic conditions. The analysis shows that, despite the loss in the configurational entropy due to the island formation, the islands containing 10-20 Li defects are present on the surface at relevant temperatures (900- 1000 K). Within the islands, the oxygen vacancy formation energy is greatly decreased due to an electron transfer from the O vacancy state to the lower energy states near the top of the valence band, associated with the Li defects.—[1] 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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