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First-principles study of intermixing and polarization at the $DyScO_3$ /$SrTiO_3$ interface KOUROSH RAHMANIZADEH, GUSTAV BIHLMAYER, STEFAN BLÜGEL, Peter Gruenberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Juelich and JARA, 52425 Juelich, Germany, MARTINA LUYSBERG, Peter Gruenberg Institut (PGI-5) & Ernst Ruska Centre, Forschungszentrum Juelich and JARA, 52425 Juelich, Germany — Exploring oxide interfaces is an attractive challenge, due to the emerging novel behaviors which don't exist in the corresponding parent bulk compounds. E. g. joining two simple band insulators $LaAlO_3$ and $SrTiO_3$ with different polarity can induce conductivity at the interface. We carried out density functional theory (DFT) calculations based on the full potential linearized augmented planewave (FLAPW) method as implemented in the `FLEUR` code (www.flapw.de) for studying the polar to non-polar interface of $DyScO_3$ and $SrTiO_3$. Due to the polar discontinuity, arising from nominally charged DyO or ScO_2 layers, sharp interfaces induce a strong ferroelectric-like polarization in the $SrTiO_3$, while in off-stoichiometric interfaces this discontinuity is avoided and no such polarization can be found. In both scenarios the interface remains insulating with only a small reduction of the bandgap. Our calculations show that chemically mixed interfaces are energetically more favorable than sharp ones. Our DFT calculations explore also different configurations of the Dy and Sr atoms within the mixed interface plane. The calculated ground state configuration is confirmed by experimental observations.

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