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Spin-texture induced by oxygen vacancies in Strontium perovskites (001) surfaces: A theoretical comparison between $SrTiO_3$ and $SrHfO_3$ MAIA VERGNIORY, Donostia International Physics Center, ANDRS-CAMILO GARCA-CASTRO, ERIC BOUSQUET, Physique Thorique des Matriaux, Universit de Lige, B-4000 Sart-Tilman, Belgium, ALDO HUMBERTO ROMERO, Physics Department, West Virginia University, WV-26506-6315, Morgantown, USA — The electronic structure of $SrTiO_3$ and $SrHfO_3$ (001) surfaces with oxygen vacancies is studied by means of first-principles calculations. We reveal how oxygen vacancies within the first atomic layer of the $SrTiO_3$ surface (i) induce a large antiferrodistortive motion of the oxygen octahedra at the surface, (ii) drive localized magnetic moments on the Ti–3d orbitals close to the vacancies and (iii) form a two-dimensional electron gas localized within the first layers. The analysis of the spin-texture of this system exhibits a splitting of the energy bands according to the Zeeman interaction, lowering of the Ti–3d_{xy} level in comparison with d_{xz} and d_{yz} and also an in-plane precession of the spins. No Rashba-like splitting for the ground state neither for ab initio molecular dynamics trajectory at 400K is recognized as suggested recently by A. F. Santander-Syro *et al.* [**?**]. Instead, a sizeable Rashba-like splitting is observed when the Ti atom is replaced by a heavier Hf atom with a much larger spin-orbit interaction. However, we observe the disappearance of the magnetism and the surface two-dimensional electron gas when full structural optimization of the $SrHfO_3$ surface is performed. Our results uncove

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