Ab initio calculations of point defects as well as (001), (011) and (111) surfaces in ABO_3 perovskites

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The review of results of surface relaxations, energetics and bonding properties for ABO_3 perovskite (001), (011) and (111) surfaces is presented [1-4]. For all ABO_3 perovskites, their (001) surface energies are quite similar. In contrast, different terminations of the (011) surface lead to very different surface energies. According to the results of calculations for Nb doped $SrTiO_3$, Nb is a shallow donor [5]. The F center in ABO_3 perovskites resembles electron defects in the partially covalent SiO_2 [6]. The results of calculations of hole and electron polarons in ABO_3 perovskites are analyzed [1,7].

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