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Half-metallicity in a $BiFeO_3/La_{\frac{2}{3}}Sr_{\frac{1}{3}}MnO_3$ heterostructure: A first-principles study[1] JILILI JIWUER, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia, ULRICH ECKERN, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We present first principles results for the electronic, magnetic, and optical properties of the $BiFeO_3/La_{\frac{2}{3}}Sr_{\frac{1}{3}}MnO_3$ heterostructure as obtained by spin polarized calculations using density functional theory. The electronic states of the heterostructure are compared to those of the bulk compounds. Structural relaxation turns out to have only a minor impact on the chemical bonding, even though the oxygen octahedra in $La_{\frac{2}{3}}Sr_{\frac{1}{3}}MnO_3$ develop some distortions due to the interface strain. While a small charge transfer affects the heterointerfaces, our results demonstrate that the half-metallic character of $La_{\frac{2}{3}}Sr_{\frac{1}{3}}MnO_3$ is fully maintained. (Reference: EPL, 102, 67009, 2013)

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