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Theoretical Scanning Probe Images of the (001) Surfaces of MnO and NiO MIHAIL GRANOVSKIJ, ANDREAS SCHRÖN, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — In the paramagnetic state the ground-state crystal structure of the $3d$ transition metal oxides (TMOs) MnO and NiO is given by an ideal rock-salt (rs) structure. Below their respective Néel temperature, however, it is characterized by the formation of an antiferromagentic ordering AFM2 which is acompanied by a rhombohedral distortion along the [111] direction. The intersection of the thermally swichable magnetic ordering AFM2 with the crystal surfaces makes TMO surfaces ideal benchmark materials for the investigation of recent magnetic scanning probe techinques such as spin-polarized scanning tunneling microscopy (SP-STM) and magnetic exchange force microscopy (MExFM). We present a density functional theory (DFT) study of the (001) surfaces of MnO and NiO inculding an on-site interaction U. Different theoretical approaches for the description of magnetic scanning probe techniques are employed. the magnetic tip is modelled by a single Fe or 5-Fe-atom pyramid. For NiO, the calculated scanning probe images explain the spin contrast and the corrugation found experimentally. For MnO, the calculated images represent interesting predictions which differ from that of NiO.

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