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Local atomic structure of the layered compound $SrFeO_2$ KAZUMASA HORIGANE, Department of Physics, Univeristy of Virginia, ANNA LLOBET, Los Alamos National Laboratory, KEESEONG PARK, DESPINA LOUCA, Department of Physics, Univeristy of Virginia — $SrFeO_2$ exhibits several unexpected structural and physical properties. Its antiferromagnetic transition temperature T_N=473K is unusually high for a two-dimensional layered structure. First-principle calculations on $SrFeO_2$ showed that the Fe 3d down-spin elections occupy the non-degenerate d_{z2} level rather than the degenerate (d_{xz}, d_{yz}) levels. This is in good agreement with the absence of a Jahn-Teller instability and the existence of the three dimensional antiferromagnetic ordering because the out-of plane direct Fe-Fe exchange is comparable in strength to the in-plane Fe-O-Fe superexchange. Therefore, it is expected that there is no structure instability in $SrFeO_2$. Using the pair distribution function (PDF) analysis to characterize the local structure of $SrFeO_2$, we observed that the local symmetry is lower than the average P4/mmm crystal symmetry. In particular, the FeO_2 planes are buckled, with two unique buckling angles along the a-axis. The buckling angle of Fe-O-Fe is reduced from $180^o$with increasing temperature, accompanied by a reduction of the Fe magnetic moment. Thus the local structure instability correlates with the magnetism where the distortions suppress orbital overlap.

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