Orbital occupation at LMO/SMO interfaces using Exact Diagonalization techniques

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We use a combined Monte Carlo / Exact diagonalization technique to investigate a spin orbital model for LMO/SMO interfaces. The model takes correlations between the Mn orbitals as well as long-range Coulomb repulsion fully into account. At the interface, we find a tendency to orbital polarization with electrons predominantly in the $3z^3-r^2$ orbital. This ferro-orbital order competes with charge order and alternating orbital order, depending on the model parameters. Similarly, spin superexchange is partly frustrated, leading to a competition between antiferromagnetic and ferromagnetic correlations.