First-order metal-insulator transitions in vanadates from first principles

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Materials that exhibit first-order metal-insulator transitions, with the accompanying abrupt change in the conductivity, have potential applications as switches in future electronic devices. Identification of materials and exploration of the atomic-scale mechanisms for switching between the two electronic states is a focus of current research. In this work, we search for first-order metal-insulator transitions in transition metal compounds, with a particular focus on d^1 and d^2 systems, by using first principles calculations to screen for an alternative low-energy energy state having not only a electronic character opposite to that of the ground state, but a distinct structure and/or magnetic ordering which would permit switching by an applied field or stress. We will present the results of our investigation of the perovskite compounds $SrVO_3$, $LaVO_3$, $CaVO_3$, YVO_3, $LaTiO_3$ and related layered phase, including superlattices and Ruddlesden-Popper phases. While the pure compounds do not satisfy the search criteria, the layered phases show promising results.