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First-order metal-insulator transitions in vanadates from first principles ANIL KUMAR, KARIN RABE, Dept of Physics and Astronomy, Rutgers University — 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 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.

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