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Prediction of ferroelectric order in $PbCrO_3$[1] MARTIN SCHLIPF, MARJANA LEŽAIĆ, Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — In this contribution, we employ density-functional theory (DFT) to analyze the properties of $PbCrO_3$. Experimental observations indicate that $PbCrO_3$ exhibits a semiconducting ground state and crystallizes in a perfect cubic perovskite structure. However, symmetry considerations show that these two properties conflict with each other and as a consequence prior DFT calculations obtained a metallic ground state. Investigating tiltings and Jahn-Teller distortions of the oxygen octahedra with a DFT+U approach, we find a semiconducting ground state in which a polar shift of the ions is energetically favorable. Depending on the size of the Hubbard U parameter, we obtain either a structure with a $P4bm$ or one with a $P4_2mc$ space group. In the $P4bm$ structure, the mechanism driving the polar displacement is analogous to $PbVO_3$. The $P4_2mc$ structure is characterized by a displacive ferroelectic order caused by empty sp orbitals.

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