Prediction of ferroelectric order in PbCrO$_3$\(^1\) MARTIN SCHLIPF, MARJANA LEŽAIČ, 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 $P4_{2}2mc$ space group. In the $P4bm$ structure, the mechanism driving the polar displacement is analogous to PbVO$_3$. The $P4_{2}2mc$ structure is characterized by a displacive ferroelectric order caused by empty $sp$ orbitals.

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