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Microscopic description of oxide perovskites and automated high-throughput analysis of their energy landscape GIOVANNI PIZZI, ANDREA CEPELLOTTI, Ecole Polytechnique Federale de Lausanne, Switzerland, BORIS KOZINSKY, Research and Technology Center, Robert Bosch LLC, Cambridge (MA), NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — Even if ferroelectric materials like $BaTiO_3$ or $KNbO_3$ have been used for decades in a broad range of technological applications, there is still significant debate in the literature concerning their microscopic behavior. For instance, many perovskite materials display a high-temperature cubic phase with zero net polarization, but its microscopic nature is though still unclear, with some materials displaying a very complex energy landscape with multiple local minima. In order to investigate and clarify the microscopic nature of oxide perovskites, we perform a study on a set of about 50 representative ABO_3 systems. We use spacegroup techniques to systematically analyze all possible local displacement patterns that are compatible with a net paraelectric phase, but can provide local non-zero ferroelectric moments. The energetics and the stability of these patterns is then assessed by combining the spacegroup analysis with DFT calculations. All calculations are managed and analyzed using our high-throughput platform AiiDA (www.aiida.net) [1]. Using this technique, we are able to describe the different classes of microscopic models underlying the perovskite systems. [1] G. Pizzi et al., Comp. Mat. Sci 111, 218-230 (2016).

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