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First principles investigation of the electro-caloric effect in $BaTiO_3$ CLAUDE EDERER, MADHURA MARATHE, Materials Theory, ETH Zurich, Switzerland — The electro-caloric effect, a change of temperature or entropy under the application of an electric field, is very promising for future applications in solid state cooling devices [1]. It has been shown that temperature changes of several Kelvin can be achieved in thin films close to the ferroelectric transition temperature [2]. However, to utilize this effect within an actual device, a good control over the caloric properties at different operating temperatures as well as a good understanding of materials-specific trends is very important. Here, we use first principles-based effective Hamiltonians [3] to study the electro-caloric effect in the prototypical ferroelectric material $BaTiO_3$. In particular, we assess the effect of epitaxial strain, which is likely to occur in thin film devices, on the caloric properties, and we show that the electro-caloric effect is quite sensitive to such epitaxial strain. We also compare direct and indirect determination of the adiabatic temperature change. The latter uses a Maxwell relation that relates the electro-caloric and pyroelectric effects. [1] J. F. Scott, Annu. Rev. Mater. Res. 41, 229 (2011). [2] Mischenko et al., Science 311, 1270 (2006). [3] Nishimatsu et al., Phys Rev. B 78, 104104 (2008).

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