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**Enhanced Piezoelectricity from Polarization Rotation in Perovskites**[1]

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Theoretical and experimental studies show that the large electromechanical response of $PbMg_{1/3}Nb_{2/3}O_3$ (PMN)-$PbTiO_3$ (PT) and related perovskite materials is due to the ease of rotating the polarization with an electric field applied oblique to the polarization. The applied field rotates the polarization from a rhombohedral phase towards tetragonal through monoclinic. Underlying the large coupling is the large c/a strain (about 6%) of ferroelectric PT. The best materials, including the most commonly used piezoelectric material, PZT ($PbZrO_3$ (PZ)-PT) tend to be solid solutions with PT. The other endmember is typically a relaxor, such as PMN or PZN. Is the relaxor behavior crucial to obtaining large coupling transducer materials? First-principles total energy and linear response computations for PT show the surprising prediction of a pressure induced morphotropic phase transition from tetragonal to monoclinic to rhombohedral, and finally cubic. In the transition regions the dielectric constant and piezoelectric constants become very large, in fact larger than those of the new single crystal piezoelectrics PMN-PT and relatives. This shows that large strain piezoelectricity in solutions with PT is due to the behavior of PT itself, and the other components simply tune the transition to zero pressure. This suggests that the key to finding new materials is in finding new pure compounds with pressure induced morphotropic phase transitions. First-principles and multiscale simulations will be discussed for relaxor ferroelectrics. This work was done in collaboration with A. Asthagiri, Y. Lei, M. Sepliarsky., Z. Wu and X. Zeng.

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