A way to search for new smart materials with unprecedented physical properties

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These thoughts begin with the observation by physicists, probing new phenomena through the use of first principles' studies, that the simultaneous occurrence of ferromagnetism and ferroelectricity is unlikely. While these studies do not consider the possibility of a phase transformation, there is a lot of indirect evidence that, if the lattice parameters are allowed to change a little, then one might have co-existence of "incompatible properties" like ferromagnetism and ferroelectricity. Thus, one could try the following: seek a reversible first order phase transformation, necessarily also involving a distortion, from, say, ferroelectric to ferromagnetic phases. If it were highly reversible, there would be the interesting additional possibility of controlling the volume fraction of phases with fields or stress. The key point is reversibility.

Even big first order phase changes can be highly reversible (liquid water to ice, some shape memory materials), and we argue that it is the nature of the shape change that is critical. We suggest, based on a close examination of measured hysteresis loops in various martensitic systems, that reversibility is governed by the presence of certain special relations among lattice parameters. We give a example of the systematic use of these relations to discover new low hysteresis shape memory materials.

Besides ferroelectricity – ferromagnetism, there are many potential property pairs that exhibit lattice parameter sensitivity and are candidates for the proposed strategy: soluability for H_2, optical nonlinearity, high band gap – low band gap semiconductors, insulator – conductor (electrical or thermal), opaque – transparent (at various wavelengths), high – low index of refraction, luminescent – nonluminescent, and new kinds of thermoelectric and thermomagnetic materials.