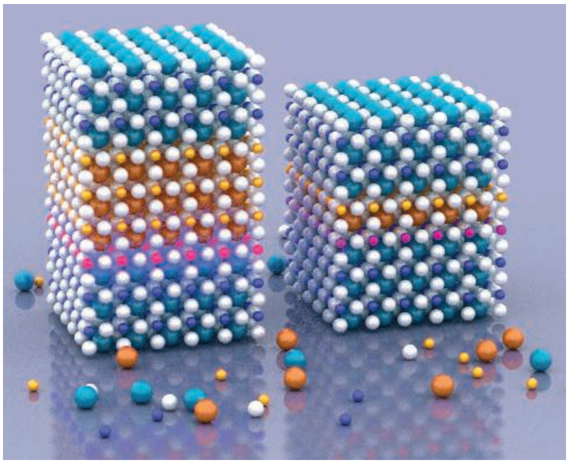
PHYSICS

When Oxides Meet Face to Face

New devices may be possible once we understand the interface between oxide materials such as superconductors and ferromagnets.

Elbio Dagotto

Multilayer structures have emerged as a leading research topic now that atomically precise methods for preparing them are available. In particular, researchers expect that oxide multilayers may lead to interesting artificial materials with novel properties (see the figure). Several of the oxides used in these multilayer systems belong to a family of compounds with strongly correlated electrons. The exotic properties of these oxides include high–transition temperature (T_c) superconductivity, with critical temperatures far higher than in standard superconductors, and colossal magnetoresistance (CMR), where the application of magnetic fields of a few teslas changes the resistivity by orders of magnitude. On page 1114 of this issue, Chakhalian *et al.* (*1*) report x-ray analysis and calculations of the interface between two such oxides.



Oxide interfaces. Models of heterostructures of lanthanum aluminate between strontium titanate layers. The atoms are represented by colored spheres (oxygen, white; lanthanum, orange; aluminum, yellow; strontium, large blue; and titanium, small dark blue). Although the materials alone are insulating, the electrical conductivity of the bottom interface (purple spheres, brighter on the left indicating higher conductivity) can be tuned due to coupling with the top interface (*11*).

These authors prepared a heterostructure with layers of (Y,Ca)$Ba_2Cu_3O_7$ (YBCO) and $La_{2/3}Ca_{1/3}MnO_3$ (LCMO) and observed a transfer of charge from the Mn oxide to the Cu oxide. This induces important modifications in the electronic orbitals of the atoms at the interface. For example, the orbitals designated $d_{3z^2-r^2}$ (*2*) are considered irrelevant in bulk cuprates because they are fully occupied and cannot act as bridges for current flow. At the interface, however, they become partially occupied and can move electrons between the two oxides. The interfacial orbitals undergo "reconstruction"—that is, they are deformed from their normal shape so that the electronic structures of the two different oxides can blend. Most of the oxides under consideration for heterostructures are very sensitive to reconstruction, something that must be considered in all future designs of artificial oxide multilayers.

High-T_c superconductivity and CMR are examples of "emergent" phenomena—new properties that cannot be anticipated from the local interactions among the electrons, and between electrons and the lattice. Many recent investigations have revealed the complex nature of these materials in bulk. These hard ceramic materials seem to hide a "soft" electronic component that produces nonlinear responses to small perturbations, as well as emergent behavior (*3*, *4*).

Artificial thin-film oxide structures could thus make the already complex individual properties of bulk strongly correlated oxides even more interesting. The oxides used in these structures could have different bulk properties, but they all have similar lattice constants (i.e., distances between atoms), allowing for a good match at the interfaces. The number of combinations of these oxides is enormous, and the potential for novel behavior is a strong motivation for these investigations.

If interfaces of semiconductors—which are rather featureless materials with a nonmagnetic rigid lattice—can nonetheless lead to fascinating physics such as the quantum Hall effect, imagine what could be done with oxides. A variety of exotic two-dimensional electronic systems could be stabilized at the oxide interfaces, exploiting spin, charge, and orbital interactions as well as lattice vibrations. Recent investigations have already shown that both a metal (*5*) and a superconductor (*6*) can be induced at the interface of two insulating materials, and the number of surprises will surely continue to grow.

Charge transfer at oxide interfaces (*1*, *7*) produces novel two-dimensional phases, as well as charge doping without the typical disorder caused by chemical doping. Thus, interfaces provide an interesting venue for doping oxide perovskites (such as the high-T_c materials) with carriers (*8*). Technological applications are also possible. For example, several groups are working on compositionally graded interfaces made from manganites with the hope of achieving high-performance magnetic tunneling junctions (*9*).

The field of "oxide electronics" is growing fast (*10*), although achieving the mobility levels and purity seen in semiconductor heterostructures remains a challenge. The combination of all these issues is what makes oxide heterostructures so interesting: This area of research is located at the intersection between fundamental science investigations and technological applications.

Previous studies of oxide heterostructures were framed in terms of "lattice reconstruction." That is, because interfacial ions are subject to forces different from those in bulk, these atoms can change position. And the mere transfer of charge at interfaces can lead to "electronic reconstruction" (*7*, *11*). In this case, the different electronic density at the interface relative to the bulk is the origin of the exotic properties. Chakhalian *et al.* have now introduced orbital reconstruction as a third process. Although the $d_{3z^2-r^2}$ orbital is widely thought to be unimportant in bulk cuprates, it is known to be crucial in bulk manganites. As cluster calculations suggest (*1*), the reported strong Cu-O-Mn bond that leads to the orbital reconstruction is precisely caused by the $d_{3z^2-r^2}$ orbital becoming active on both sides of the interface.

Despite recent activity, the field of oxide interfaces remains virtually unexplored. What might happen if we could mix materials with vastly different properties such as ferromagnets, antiferromagnets, superconductors, ferroelectrics, multiferroics, geometrically frustrated spin systems, heavy fermions, and others? Considering this enormous number of combinations, theoretical guidance is needed. But for theory to be useful, the calculations must be reliable, at least qualitatively. Powerful techniques are needed to study inter-

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faces of strongly correlated electronic systems. Reliable procedures to calculate and measure work functions of individual materials are also needed to predict the direction of charge transfer at interfaces. The collective responses and nonlinearities of models for oxide interfaces must be carefully analyzed. By this multilevel effort, the potential new functionalities and exotic phases of the oxide combinations under scrutiny will hopefully be revealed. Lattice, electronic, and now orbital reconstructions will all be essential in the effort to understand and use oxide interfaces.

References and Notes

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GENETICS

Widespread Monoallelic Expression

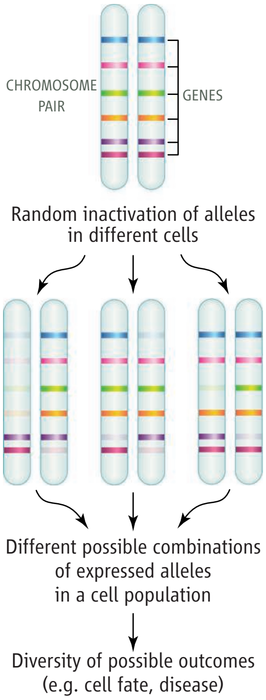
The surprisingly high prevalence of random allele inactivation in human cells can generate diversity in gene expression that affects cell fate and physiology.

Rolf Ohlsson

Most eukaryotic cells have two copies of autosomal (non–sex-determining) chromosomes. Although both copies (alleles) of individual genes are usually expressed in each diploid cell, one of the alleles is inactivated in a subset of genes (*1*). It is of profound interest that monoallelic expression in somatic cells does not simply represent a rheostat control for gene expression. Rather, it often operates in some selective function, such as determining the repertoire of odorant receptors or T cell receptors that are expressed (*2*, *3*). Moreover, the parental alleles of some mouse genes, such as those that encode cytokines, are expressed in random patterns, in which either, neither, or both alleles are inactivated, potentially influencing the selection and expansion of particular on T cells (*4*).

On page 1136 in this issue, Gimelbrant et al. (*5*) report that the mammalian genome employs random, monoallelic expression more extensively than thought. This may be to generate diversity in expression patterns on an unprecedented scale, which has important implications for the ontogeny of human diseases.

Gimelbrant *et al*. determined the proportion of human genes that can be expressed monoallelically, in patterns that are epigenetically stable (for example, chemical modifications of DNA, such as cytosine methylation, that do not alter the sequence but are heritable within cell populations). They identified expressed alleles in cloned cell populations of human B lymphocytes by taking advantage of polymorphic sequences, or single-nucleotide polymorphisms (SNPs). By modifying a method for detecting SNPs in DNA sequences, Gimelbrant *et al*. were able to track expressed messenger RNA (mRNA) sequences. Because most of the SNPs for the 3939 genes that were assessed are located in noncoding introns that are not present in mature mRNA, the authors included precursor forms of mRNAs (which contain introns) in the samples that were analyzed. They identified 371 genes (nearly 10%) as monoallelically expressed in epigenetically stable patterns in at least one population of cells derived from a single B cell clone. Although most of these genes were also found to be biallelically expressed in some other B cell populations, up to 20% could be consistently expressed from one of the parental alleles in some B cell clones. Thus, each cell population displays a vast heterogeneity in patterns of mono- and biallelic gene expression, providing numerous combinatorial patterns of gene expression (see the figure).



Generating diversity. Alleles are randomly inactivated on a pair of chromosomes in a human somatic cell. The various patterns of inactivation in progeny cells are then stabilized (epigenetically). This can generate diverse cellular and physiological outcomes.

Although other patterns of monoallelic expression have been described in human cells (*6, 7*), Gimelbrant *et al*. go much further in two important respects. First, they analyze a large number of genes, thereby increasing the generality of their conclusions. Indeed, based on their findings, the authors argue that more than 1000 genes in the human genome can potentially be monoallelically expressed at any given time, indicating an amazing degree of diversity in possible combinations of expressed alleles. Interestingly, genes encoding cell surface receptors are overrepresented in this subset, suggesting the enormous potential for epigenetic regulation of receptor-mediated cell-cell communications, and hence, the regulation of cell diversity and cell fate (*8*). Second, Gimelbrant *et al*. hint at the fascinating possibility that the same set of genes can be monoallelically expressed at certain stages of development in a subset of tissue cells and/or perhaps in only some individuals.

It is unclear, though, how random monoallelic expression is established in somatic cells. Unlike the acquisition of imprinted, methylated marks on DNA from the parental germ lines–so-called genomic imprinting, which inactivates either a maternal or paternal allele during gamete development (*1*)—random inactivation of nonimprinted autosomal alleles occurs in somatic cells. Gimelbrant *et al*. show that many of the monoallelically expressed genes are highly expressed, apparently ruling

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