Rising Energy Costs

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It's rare that additional fees are welcome, but as **Steven Johnston (http://www.phys.utk.edu/faculty/faculty-johnston.html)** and his colleagues explain in *Nature Communications*, sometimes they can actually be a pleasant surprise. In "**Electron-lattice interactions strongly renormalize the charge transfer energy in the spin-chain cuprate Li_2CuO_2 (http://www.nature.com/ncomms/2016/160217/ncomms10563/full/ncomms10563.html)**," which appears in the February 17 issue of the journal, they report on how extra energy costs associated with the motion of electrons in lithium copper oxides reveal more about these materials, and in turn help scientists better understand their electronic properties.

Electron Hopping

The research has to do with insulators: materials that make it virtually impossible for electric current to flow. Band insulators, as Johnston explained, are your typical everyday insulators, where so many electrons are crammed into the material that there are no low-energy quantum states left for them to go into. In this case, electron motion is blocked by the fact that the electrons have nowhere to go. Mott (named for Sir Nevill Francis Mott) and charge-transfer insulators are a bit different. Quantum mechanical calculations indicate these insulators should be conductors, where current moves freely. Yet their electrons—which typically repel one another—strongly interact with each other such that for one to move, another would have to get out of its way. (Johnston gave the illustration of trying to traverse a very crowded room.)

If and how current moves is a key property of the insulators, semiconductors, and superconductors that drive the electronics industry. Among the materials that cover the breadth of this territory are the transition metal oxides, which are built from repeated blocks of transition metal ions surrounded by oxygen atoms. In these materials, electrons can move along one of two pathways: they can either hop from metal ion to metal ion or, alternatively, they can hop from the metal ion to one of the oxygen atoms and then subsequently to neighboring oxygen atoms. In most transition metal oxides, both of these alternatives cost energy, thus making them insulators; however, which of these two pathways is most desirable determines the classification of the insulator. In a Mott insulator the hopping between the metal ions is cheaper in terms of energy cost. Conversely, in a charge transfer insulator, the hopping to the oxygen sublattice is. This classification scheme dates to 1985 when it was first proposed by Zaanen, Sawatzky, and Allen. Since then, the prevailing opinion has been that the relevant energy scales were determined by the local chemistry of the material. This paper in *Nature Communications* shows it's a bit more sophisticated than that.

Hidden Fees

Scientists began with the charge transfer insulator lithium copper oxide. Using computer modeling and resonant inelastic x-ray scattering (RIXS) they were able to see a much more complex picture. They found that not only is there an electronic energy cost required for electrons to hop to oxygen sites, but there's also an additional energy cost caused by movement of the material's crystal structure, or lattice. In the case of Li_2CuO_2, they found that the interaction of electrons with the lattice vibrations is responsible *for more than half* of the charge transfer energy. This paper is the first observation of the charge transfer energy being significantly influenced by the motion of the lattice.

Johnston explained that with any given material, understanding where it belongs is a good start for understanding its basic properties. Electrons want to move along the path of least resistance. Therefore, whichever pathway has the lower energy cost will determine how the insulator will behave when subjected to perturbations like electric fields.

“What can dictate these energy scales is much broader than we originally thought,” he said.

The *Nature Communications* research gives scientists more options for classifying materials and will be relevant for a number of low-dimensional materials, a class that includes high-temperature superconductors, nanotubes, and quantum dots.

Johnston’s colleagues on the paper include Claude Monney, Valentina Bisogni, Ke-Jin Zhou, Roberto Kraus, Günter Behr, Vladimir N. Strocov, JiriMálek, Stefan-Ludwig Drechsler, Jochen Geck, Thorsten Schmitt, and Jeroen van den Brink. They represent the Paul Scherrer Institut (Switzerland), the Institute of Physics at the University of Zurich, the Leibniz Institute for Solid State and Materials Research (Germany), the National Synchrotron Light Source II at Brookhaven National Laboratory, and the Institute of Physics, ASCR (Czech Republic).