

S. Trippel of the University of Freiburg in Germany, E. Hamilton at Northwestern University, and their colleagues have reported in the October 5, 2007 issue of *Physical Review Letters* (DOI:10.1103/PhysRevLett.99.143602) an effective method to control the alignment and rotation of molecular objects using synchronized nanosecond and femtosecond laser pulses. The researchers also used quantum mechanical simulations to support their experimental findings on the efficacy of their method to align and manipulate molecules.

Laser alignment of molecules results

from the interaction of the laser pulse with the dipole moment of the molecule. The research team employed a 10 nanosecond duration laser pulse to align molecules of 3,5 difluoriodobenzene (DFIB) along its most polarizable axis (the axis defined by the bond between the C and I atoms). They then applied an orthogonally polarized 150 femtosecond duration pulse to activate motion about the aligned axis, resulting in rotation. The orientation and movement of the molecules was measured by monitoring ion fragments released from the molecules through pulsed excitation, as shown in Figure 1. By varying the length and

strength of the nanosecond and femtosecond alignment pulses, the researchers uncovered a parameter space within which the behavior of the molecule could be controlled. A numerical solution based on a nonperturbative solution of the Schrödinger equation of the molecular dipole and two laser fields provided a quantum mechanical basis for describing the behavior of the molecule.

Though these experiments were carried out on 3,5 difluoriodobenzene, the researchers generalized their model for an arbitrary molecular system. Furthermore, they expect, based on their numerical calculations, that by applying more sophisticated pulse sequences to the molecule, field-free alignment will be achieved. This method could prove fruitful for investigations exploring the rotational dynamics of complex molecules as well as for control of molecular torsions.

ARTHUR FELDMAN

Cooperative Conduction Mechanisms Determined for Candidate Fuel Cell Electrolyte

Fuel cells are gaining increased attention recently as an efficient and clean method of generating electricity. An example is the solid-oxide fuel cell, where *solid oxide* refers primarily to the materials used for the electrolyte, and good conduction paths for O^{2-} or H^+ ions are required. Optimizing the conductivity in the electrolyte can significantly increase the overall efficiency of the cell. The novel oxide $La_{1-x}Ba_{1+x}GaO_{4-x/2}$ is a promising candidate electrolyte in the emerging class of proton-conducting ceramics, due to its intermediate operating temperature, 500–700°C, and the high conductivities of both oxygen ions and protons. E. Kendrick and P.R. Slater of the University of Surrey, J. Kendrick of the University of Bradford, K.S. Knight of CCLRC Rutherford Appleton Laboratory and the Natural History Museum, and M.S. Islam of the University of Bath have determined the unusual conduction mechanisms in this system through a combined experimental and computational approach, a vital step toward optimizing the conductivity. They published their findings in the November 2007 issue of *Nature Materials* (p. 871, DOI:10.1038/nmat2039).

Unlike the perovskite and fluorite compounds typically used in solid-oxide fuel cells, $La_{1-x}Ba_{1+x}GaO_{4-x/2}$ has tetrahedral structural units, where the Ga atom is surrounded by a group of four oxygen ions in a tetrahedral configuration. The researchers found that this structure is key to the mechanism by which oxide ions move through the lattice. They discovered that an oxygen vacancy is accommodated

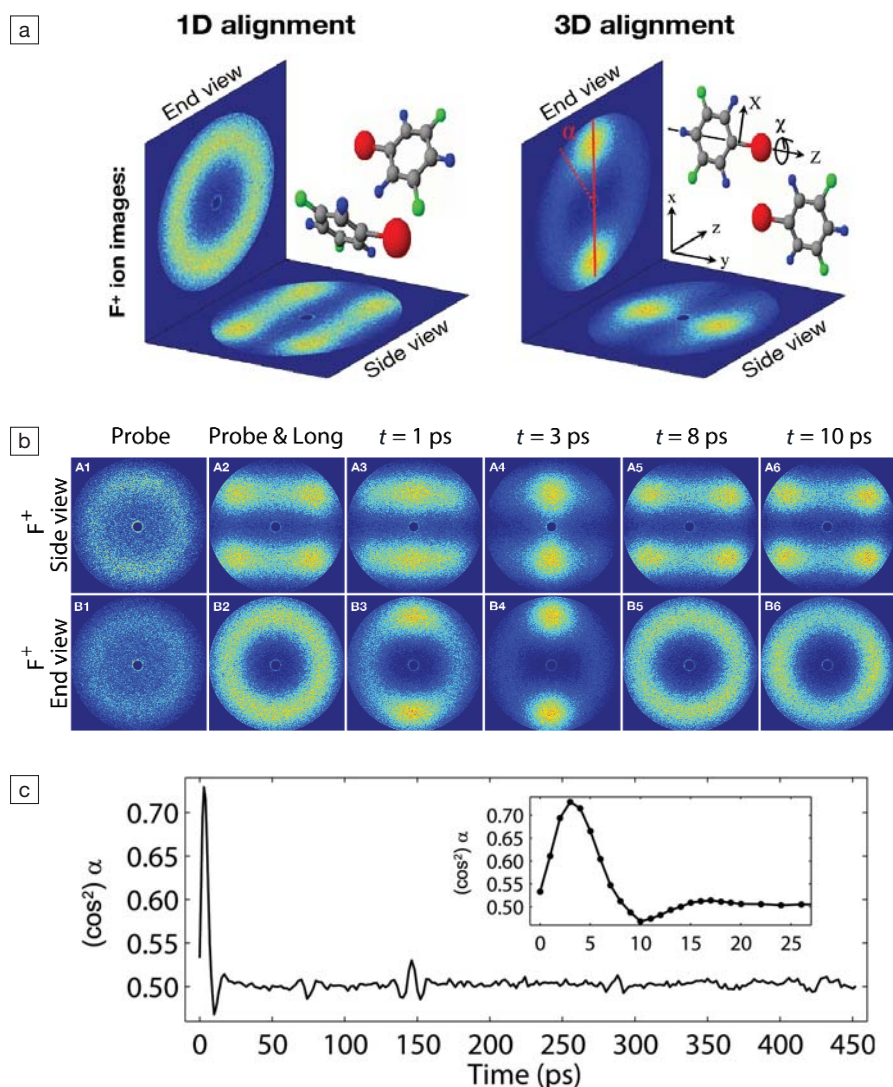


Figure 1: An overview of the laser pulse molecule alignment technique. (a) F^+ ion imaging of 3,5 difluoriodobenzene (DFIB) shows alignment in one and three dimensions, respectively, with the coordinate system shown in red. (b) Time-lapsed F^+ ion imaging of DFIB shows the dephasing and revival of 3D alignment. (c) Stimulated rotation of the molecule, as measured by the expectation value of the angle of rotation about the tightly aligned molecular axis $(\cos^2) \alpha$, shown as a function of time after the short pulse. Reprinted with permission from *Physical Review Letters* **99** (2007) 143602. ©2007 by the American Physical Society.

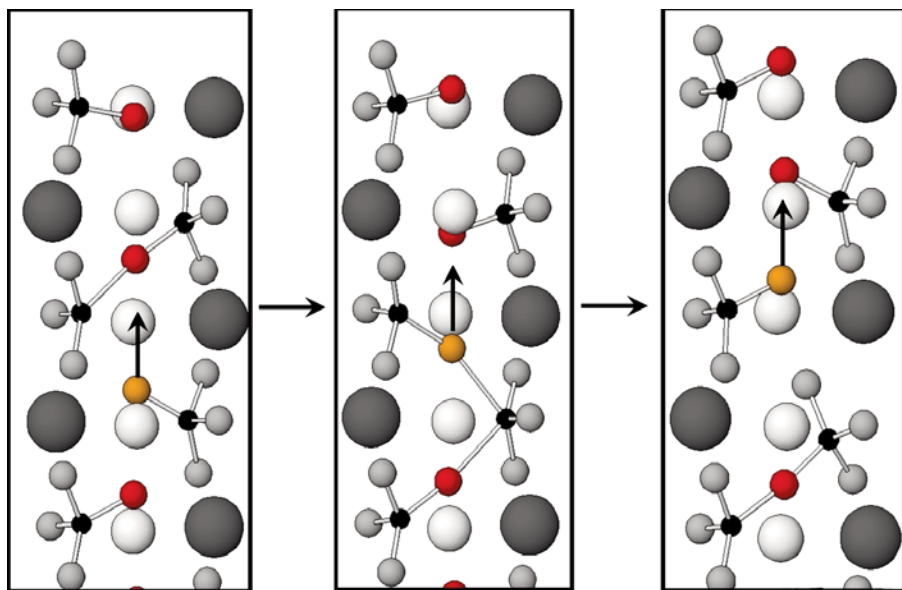


Figure 1. Snapshots taken from simulations show the microscopic mechanism of oxide-ion migration involving the formation and breaking of Ga_2O_7 units. The migrating oxide ions are highlighted, and the stick bonds are drawn to aid the interpretation of the transport mechanism. Reprinted by permission from Macmillan Publishers Ltd: *Nature Materials* 6 (November 2007) 871, © 2007.

by the distortion of a neighboring GaO_4 tetrahedron, creating a Ga_2O_7 unit in which both Ga atoms are still tetrahedrally coordinated. A "cog-wheel" type process

then passes the vacancy along (see Figure 1) as Ga_2O_7 units form and break in cooperation. The diffusing O ions thus take a path that is anisotropically directed along


the c axis, relying on the easy rotation of the oxygen tetrahedra, spurring the cog-wheel analogy. The researchers used atomistic modeling of the local structure to predict the presence of these Ga_2O_7 units and confirmed their existence by re-examining neutron diffraction data. They investigated the diffusion behavior, using potential-based simulations in which the lattice was allowed to relax around the migrating ion, as well as molecular dynamics simulations.

At lower temperatures, proton conduction dominated. Protons were introduced into the lattice by incorporation of water, eliminating oxygen vacancies and breaking up the Ga_2O_7 units. The researchers studied the movement of a proton in the lattice using density functional theory (DFT) calculations. By comparing activation energies, they determined that the rate-limiting step for proton diffusion is the movement of the proton around a given tetrahedra, while movement between neighboring tetrahedra is comparatively easy. Unlike the oxygen vacancies, proton diffusion is isotropic, with inter-tetrahedral proton transfer occurring equally easily in all directions. The researchers said, "this mechanistic understanding of proton and oxide ion conduction may lead to fuel cells of increased efficiency using electrolytes based on LaBaGaO_4 or related compounds."

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