Independent control of ionic and electronic conductivity research

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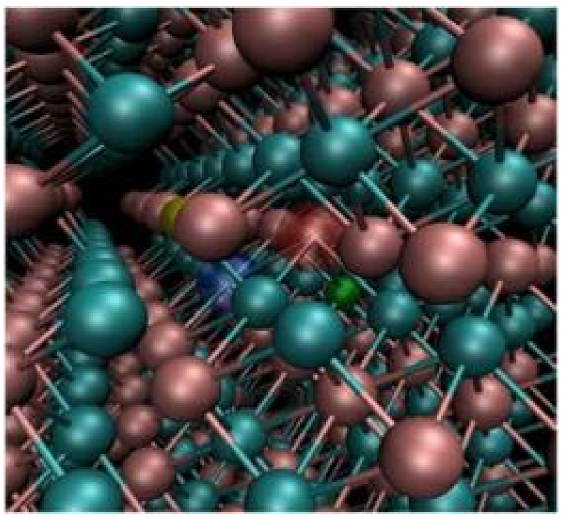

Atomic structure of co-dopant complex in thallium bromide that binds charged vacancies and reduces their mobility, allowing selective control over ionic conductivity without affecting electronic conductivity.

(Phys.org) -- Lawrence Livermore National Laboratory researchers have discovered a new method to control the conductivity of materials that could eventually apply to fuel cells, batteries and gas sensors.

Postdoc Cedric Rocha-Leão, working with Condensed Matter and Materials Division's Vince Lordi, has found a new method to independently control ionic and electronic conductivities in certain solids.

The method, which uses tailored acceptor-donor co-doping to bind charged native vacancies and selectively modulate ionic but not electronic conductivity, was developed by using first-principles materials simulations.

The computational materials design approach allowed quantitative screening of dopants to find those most effective for a particular application. Their recent work focused on optimizing conduction in thallium bromide for high-resolution room-temperature gamma radiation detectors, for which high electronic conductivity and low ionic conductivity are required.

Achieving simultaneous control of ionic and electronic conductivity in materials is one of the great challenges in solid state ionics. Since these properties are intertwined, optimizing one often results in degrading the other.

But the new method limits ionic current without impacting the electronic properties for a general class of materials, based on co-doping with oppositely charged ions.

The research appears in the June 15 edition of *Physical Review Letters.*

Provided by Lawrence Livermore National Laboratory