

Team models ionic conductivity in doped ceria for use as a fuel cell electrolyte

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(PhysOrg.com) -- Optimizing the conductivity of ceria based oxides, or doped ceria, is crucial to their use as electrolytes in future solid oxide fuel cells.

Researchers from the NIST Center for [Nanoscale Science](#) and Technology and Arizona State University have successfully used kinetic lattice [Monte Carlo simulations](#) to predict the optimum dopant concentration for maximizing [conductivity](#) for gadolinium doped ceria⁽¹⁾, and for double-doped (praseodymium and gadolinium) ceria⁽²⁾, at temperatures (773 K to 1073 K) that are practical for fuel cell operation.

Compared with the [electrolytes](#) that are commonly used in [solid oxide fuel cells](#), doped ceria has higher conductivity and therefore higher efficiency. It also operates at lower temperatures, which may reduce the overall material costs for the fuel cells.

The researchers used their previously published Monte Carlo model to calculate activation energies using density functional theory that includes electron interactions (DFT + U) in order to study time-dependent vacancy diffusion.

Their results showed that ionic conductivity is maximized between 0.2 mole fraction and 0.25 mole fraction for gadolinium and decreases slightly for higher concentrations. For the same doping concentrations, double-doped ceria had higher ionic conductivity than single-doped, with

gadolinium-rich double-doped ceria having the highest conductivity.

The models explain the performance difference between double and single doping by showing that in the double-doped ceria, vacancy diffusion follows low energy migration paths.

The researchers' calculations agree with available experimental data, indicating that their model can be used to predict the behavior of other lanthanide co-dopants in ceria-based oxides.

More information: (1)Predicting the optimal dopant concentration in gadolinium doped ceria: a kinetic lattice Monte Carlo approach, P. P. Dholabhai, et al., *Modelling and Simulation in Materials Science and Engineering* 20, 015004 (2011).

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(2)In search of enhanced electrolyte materials: a case study of doubly doped ceria, P. P. Dholabhai, et al., *Journal of Materials Chemistry* 21, 18991-18997 (2011). [pubs.rsc.org/en/Content/Article...](http://pubs.rsc.org/en/Content/Article/2011/JM/c1jm14417k)

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