

第25回稲盛フロンティア研究セミナー

稲盛フロンティア研究センターでは、以下の講演会を開催します。ご参加は無料です。お気軽にご参加下さい。

日時:平成 28 年 10 月 14 日(金)16:00~17:00

場所:稲盛財団記念館 2F セミナー室



On the conductivity maximum in rare earth-doped ceria 計算科学による希土類元素添加酸化セリウムにおける 酸化物イオン導電率の最大化

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Interest in materials exhibiting oxygen ion conduction has increased during the last years owing to their great importance for energy applications, such as solid oxide fuel cells for converting chemical to electrical energy and solid oxide electrolyzer cells for high-temperature electrolysis of water.

Ceria-based oxides are regarded as key oxide materials for energy applications due to the fact that rare earth-doped ceria is a pure oxygen ion conductor, while undoped ceria is a mixed oxygen ion-electron conductor. Using density-functional theory (DFT) we have investigated defect formation energies and entropies and oxygen migration energies as well, both in undoped and in rare earth-doped ceria. The macroscopic oxygen ion conductivity was then investigated by means of Kinetic Monte Carlo (KMC) simulations. We show that all interactions between the defects, namely vacancy-dopant attraction, dopant-dopant repulsion and vacancy-vacancy repulsion as well contribute to the so-called conductivity maximum of the ionic conductivity. We also demonstrate that ordering of the cations is one source of long-term degradation of the oxygen ion conductivity.

近年、固体酸化物型燃料電池(SOFC)や高温水蒸気電解(SOEC)等の電気化学デバイスへの応用が期待され、固体電解質に用いられる酸化物イオン伝導体の研究が盛んに行われている。その中でも希土類をドーパントとした酸化セリウムにおいては、高い酸化物イオン伝導性とイオン輸率を有することから特に注目されている。本研究では、第一原理計算を用いて酸化セリウム、および希土類置換酸化セリウムにおける欠陥生成エネルギーおよび酸素拡散における活性化エネルギーを調査した。さらに、モンテカルロシミュレーションを用いてマクロなイオン伝導率の算出を行った。また本講演においては、計算により得られた全ての元素間の相互作用である、酸素空孔-ドーパント引問力、ド合わせ先-パントドーパント反発力、酸素空孔-酸素空孔反発力が酸化物イオン伝導性に及ぼす影響について示す。さらに、酸化セリウムにおける酸化物イオン伝導度の劣化がカチオンの規則化による影響であることについて見出したことを報告する。



Professor Manfred Martin

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Manfred Martin is Professor and Head of the Institute of Physical Chemistry of RWTH Aachen University, Germany, where he is also the Rector's delegate for cooperation with Korea. At Seoul National University, Korea he was WCU Professor and is now Adjunct Professor. He has more than 30 years of experience in education and research of physical chemistry of solids as well as service at department, faculty and university level. His current research focusses on materials for energy conversion, resistive switching, solid-state reactions, secondary ion mass spectrometry, and computer simulations as well. Professor Manfred Martin has published >200 scientific papers in international, refereed journals. He is organizer of a series of international conferences and symposia and is invited for plenary, keynote, and invited lectures at international conferences and symposia on a regular basis. He received the Carl-Wagner Award and has been elected as member of the Royal Society of Chemistry. He has supervised more than 50 Ph.D. students and more than 20 postdoctoral fellows. Professor Manfred Martin has won and managed a large number of research programs and grants, and he is serving in editorial boards and expert panels of Germany and overseas as well.

後援:九州大学 PROGRESS100

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