Understanding ion transport phenomena in heterostructured yttria-stabilized zirconia with respect to coordination chemistry

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Yttria-stabilized zirconia (xY -(1-x)ZrO , YSZ) has been exploited as a fast oxygen-ion conductor at elevatedtemperature, which is benefited from the formation of oxygen vacancies upon thestabilization of zirconia by yttria doping. Oxygen ion conduction in YSZ takesplace by exchanging oxygen ions and vacancies within the cubic/tetragonalcrystal framework, therefore, the coordination chemistry of a Zr ion by oxygenare of key importance in terms of crystal structure and crystal field tounderstand the origin of fast ionic conduction in YSZ. Herein, the Zr-Ometal-ligand interactions are modulated by heterostructuring of YSZ with Smdoped ceria, by which the vibrational properties of Zr-O bonding are altered.The coordination chemistry of the heterostructures is studied by X-rayabsorption spectroscopy on Zr L edges, which is combined with neutrondiffraction and inelastic neutron scattering studies. The coordinationchemistry model for the heterostructures is suggested in conjunction with abinitio calculations.