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ABSTRACT:

Hydride ion defects in barium indate zirconate perovskite

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Metal oxyhydrides, including the hydride anion (H^-), are rare but have recently become appealing hydrogenation catalysts for ammonia synthesis[1-3] and CO_2 conversion[4, 5]. H^- is simply the counter form of H^+, but the electrochemical activity of the former could clearly be distinguished from that of the latter because the high redox potential of H_2/H^-, at −2.3 V versus a normal hydrogen electrode, may facilitate electron donation to adsorbed molecules.[2, 6] The oxyhydrides must be important H^- ion conductors because the large polarizability and extraordinary ion-size flexibility of H^- anion is advantageous for the long-range diffusion. On account of the transferability and redox activity of the H^- anion, therefore, materials with significant H^- ion conductivity are promising options not only for catalytic substances but also for ceramic electrochemical devices,[7, 8] such as co-electrolysis cells[9-11] and membrane reactors,[12] Cubic perovskite type barium zirconate, $BaZr_{1-x}In_xO_{3-\delta}$ ($0<x<0.7$), have been intensively studied for their excellent proton conductivity and tolerance to high p_{H2O} atmosphere. Herein, we demonstrated that the incorporation of H^- ion defects in $BaZr_{0.5}In_{0.5}O_{2.75}$ (BZI55) in H_2 atmosphere at low water partial pressure (p_{H2O}). $BaZr_{0.5}In(III)_{0.5}O_{2.75}$, as the parent phase, was readily hydrogenated via simple H_2 gas annealing at 800 °C under ambient pressure with the reduction of In atoms and insertion of vacancies and H^- ions into O sites bridging two In atoms (O_{In}^{In}). The resultant $BaZr_{0.5}In(II)_{0.5}O_{2.25}H_{0.5}$ phase exhibited relatively high hydrogen permeability due to the mixed H^- ion/electron conductivity.

[1] H. Toriumi, G. Kobayashi, T. Saito, T. Kamiya, T. Sakai, T. Nomura, S. Kitano, H. Habazaki and Y. Aoki, Chem. Mater., 34, 7389 (2022).