**Inhibiting in situ phase transition in RuddlesdenPopper perovskite via tailoring bond hybridization and its application in oxygen permeation**

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**Abstract:**

Ruddlesden-Popper (RP, An+1BnO3n+1) oxide based mixed ionic-electronic conducting (MIEC) membranes have been proposed as a promising new cost-effective method to provide pure oxygen from air to replace the conventional expensive and energy-intensive cryogenic techniques. However, the oxygen permeability of the existing MIEC membranes is still in need to be improved due to the limited oxygen ionic and electronic conductivity or the unsatisfactory operational stability. Element-doping has been recognized as a facile and efficient strategy either to improve the oxygen ionic or electronic conductivity or to stabilize the crystal phase structure (by inhibiting both ex-situ and in-situ phase transition) favorable for oxygen permeation. Herein, the ex-situ collapse of crystal together with the generation of impurities in orthorhombic Pr2NiO4 with Mo doping are observed as the rearrangement of Pr atoms-based lattice deformation, which could be attributed to the enhanced formation energy. Noteworthy is that, Mo-doping would give rise to the inhibition of in-situ phase transition from low order Pr2NiO4 (n=1) to high order Pr4Ni3O10 (n=3) by weakening the covalent interaction of Pr-O and then promote the mobility of interstitial oxygen. An optimum doping level in Pr2Ni1-xMoxO4+δ was identified at x value of 0.05 to achieve the best oxygen separation flux. Furthermore, Pr2Ni0.95Mo0.05O4+δ membrane not only shows high permeation stability in air and helium, but also exhibits high CO2 tolerance without obvious decline on oxygen permeation flux for over 500 hours at round 900 oC. This work advances a comprehensive understanding of ex-situ and in-situ phase transition on Pr2NiO4-based RP materials and provides an effective way to enhance the oxygen permeability via Mo doping to in-situ stabilize phase structure and improve the mobility of interstitial oxygen.

**Biography of presenting author**

Dr. Ning Han is now doing research at Department of Materials Engineering, KU Leuven, Belgium. His current research is mainly lie in design and characterization of oxide-based materials with the application focus on electrocatalysis, environmental catalysis, and energy storage. Within 5 years, he has authored and co-authored over 50 scientific papers published in international journals, and 5 granted patents.

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