

Profound Understanding of Effect of Transition Metal Dopant, Sintering Temperature and pO_2 on the Electrical and Optical Properties of Proton Conducting $BaCe_{0.9}Sm_{0.1}O_{3-\delta}$

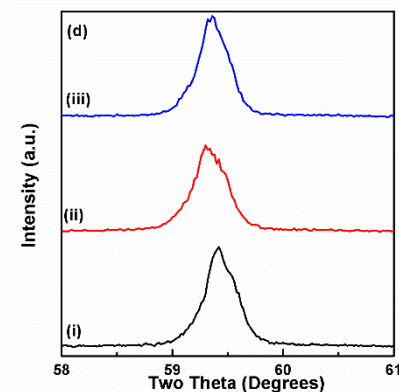
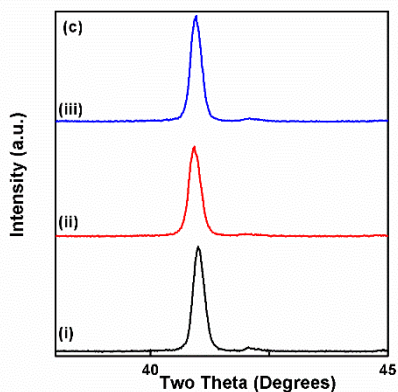
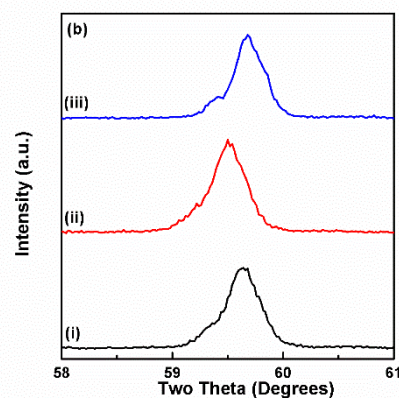
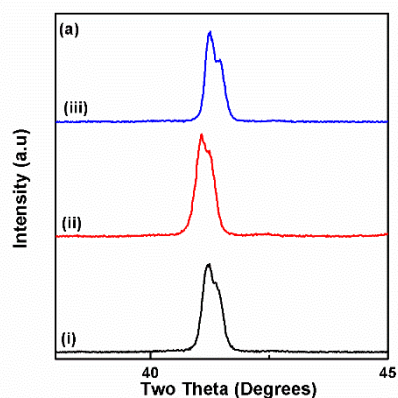
Hala T. Handal ^{a,b}, Azfar Hassan ^c, Ryan Leeson^a, Sherif M. Eloui ^b Martin Fitzpatrick ^a and Venkataraman Thangadurai^{a,*}

^a Department of Chemistry, University of Calgary, Calgary, AB, T2N 1N4 Canada

^b Department of Chemistry, National Research Centre, 12622 Dokki, Cairo, Egypt

^c Department of Chemical and Petroleum Engineering, University of Calgary, Calgary, AB, T2N 1N4 Canada *Corresponding author e-mail: vthangad@ucalgary.ca

Supporting Information



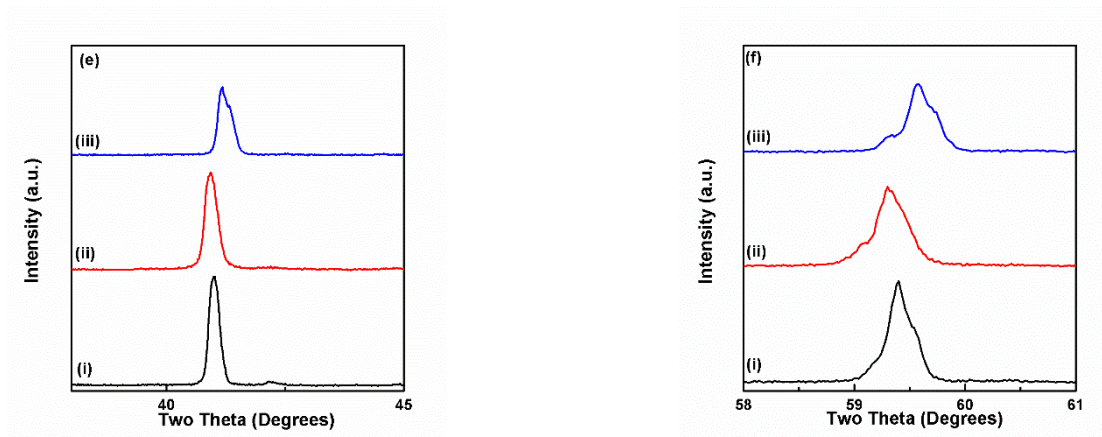


Figure S1. Magnified PXRD peaks at (400) and (132) for the two theta between 38-45° and 58-61° of (a,b) $\text{BaCe}_{0.9}\text{Sm}_{0.1}\text{O}_{3-\delta}$ (BCS), (c,d) $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Fe}_{0.05}\text{O}_{3-\delta}$ (BCSF), and (e,f) $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Co}_{0.05}\text{O}_{3-\delta}$ (BCSC) samples sintered at 1200°C for 8h and followed by annealing in (i) air, (ii) $\text{N}_2+3\%\text{H}_2\text{O}$ and (iii) dry H_2 at 1000 °C/1h.

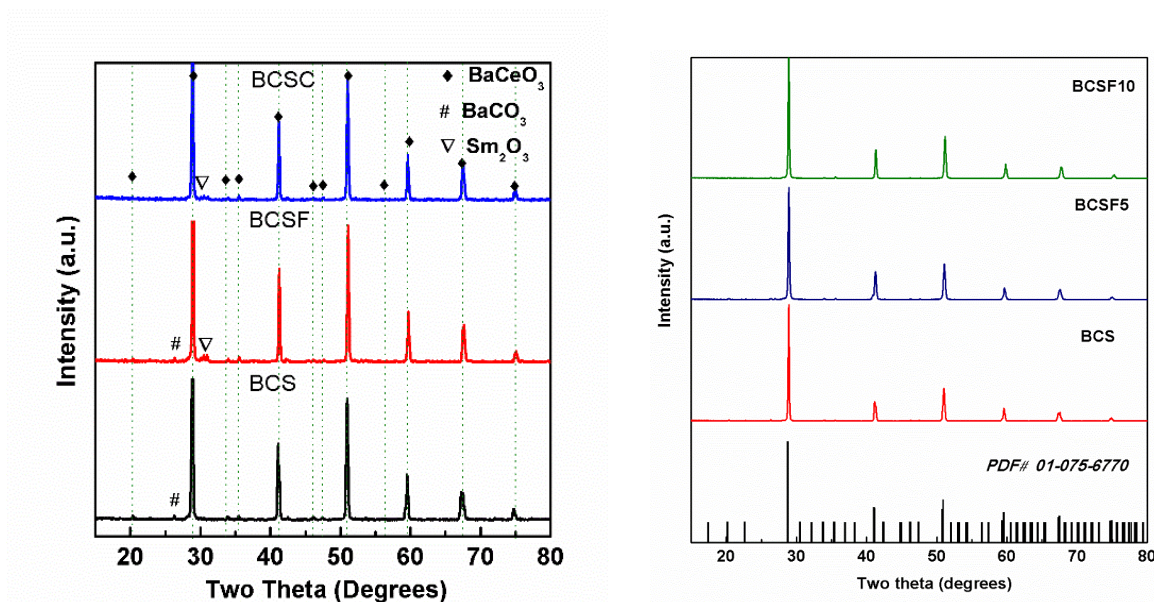


Figure S2. XRD patterns of samples sintered at (l.h.s.) 1300 °C/8h for BaCe_{0.9}Sm_{0.1}O_{3-δ} (BCS), BaCe_{0.85}Sm_{0.1}Fe_{0.05}O_{3-δ} (BCSF), and (c) BaCe_{0.85}Sm_{0.1}Co_{0.05}O_{3-δ} (BCSC), and (r.h.s.) 1400 °C/8h in ambient air for BaCe_{0.9}Sm_{0.1}O_{3-δ} (BCS), BaCe_{0.85}Sm_{0.1}Fe_{0.05}O_{3-δ} (BCSF5); BaCe_{0.8}Sm_{0.1}Fe_{0.1}O_{3-δ} (BCSF10). Phases have been recognized and indexed according to the corresponding PDF card.

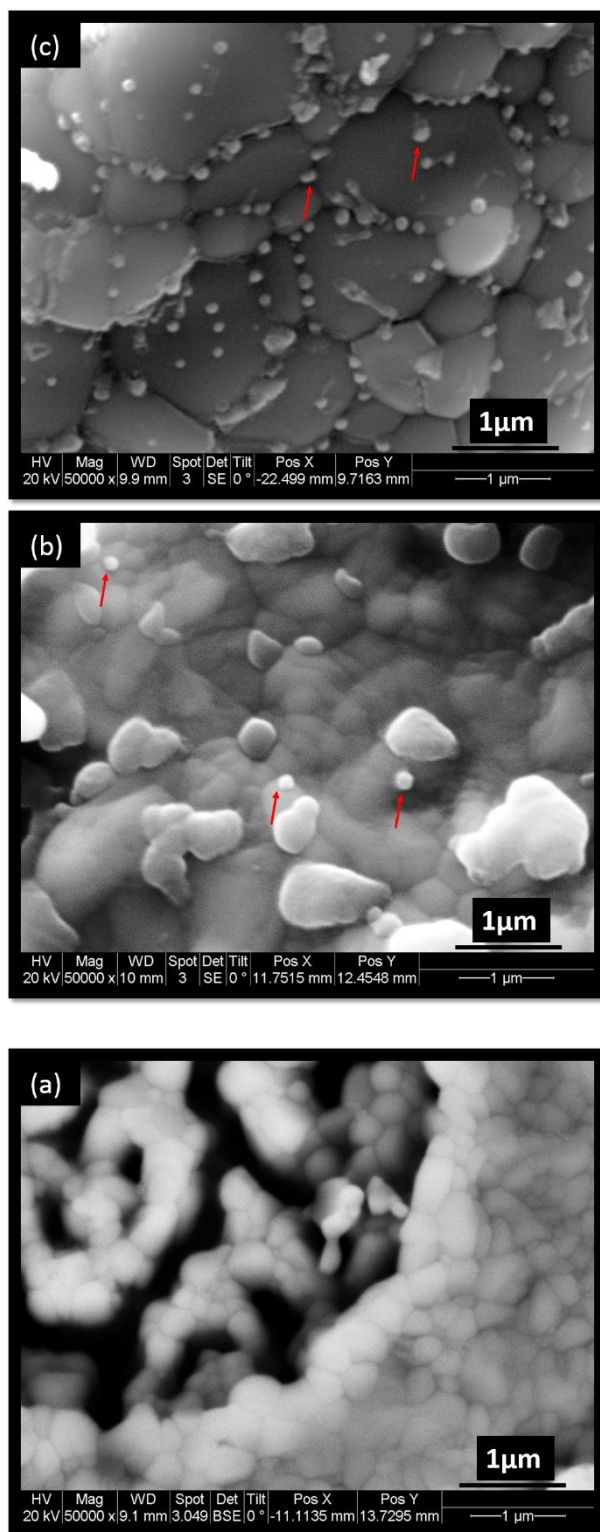


Figure S3. SEM images of (a) BaCe_{0.9}Sm_{0.1}O_{3-δ} (BCS) (b) BaCe_{0.85}Sm_{0.1}Fe_{0.05}O_{3-δ} (BCSF5) and (c) BaCe_{0.85}Sm_{0.1}Co_{0.05}O_{3-δ} (BCSC5) powder samples sintered at 1200 °C /8h in air and subsequently reduced in dry H₂ at 1000 °C/1h.

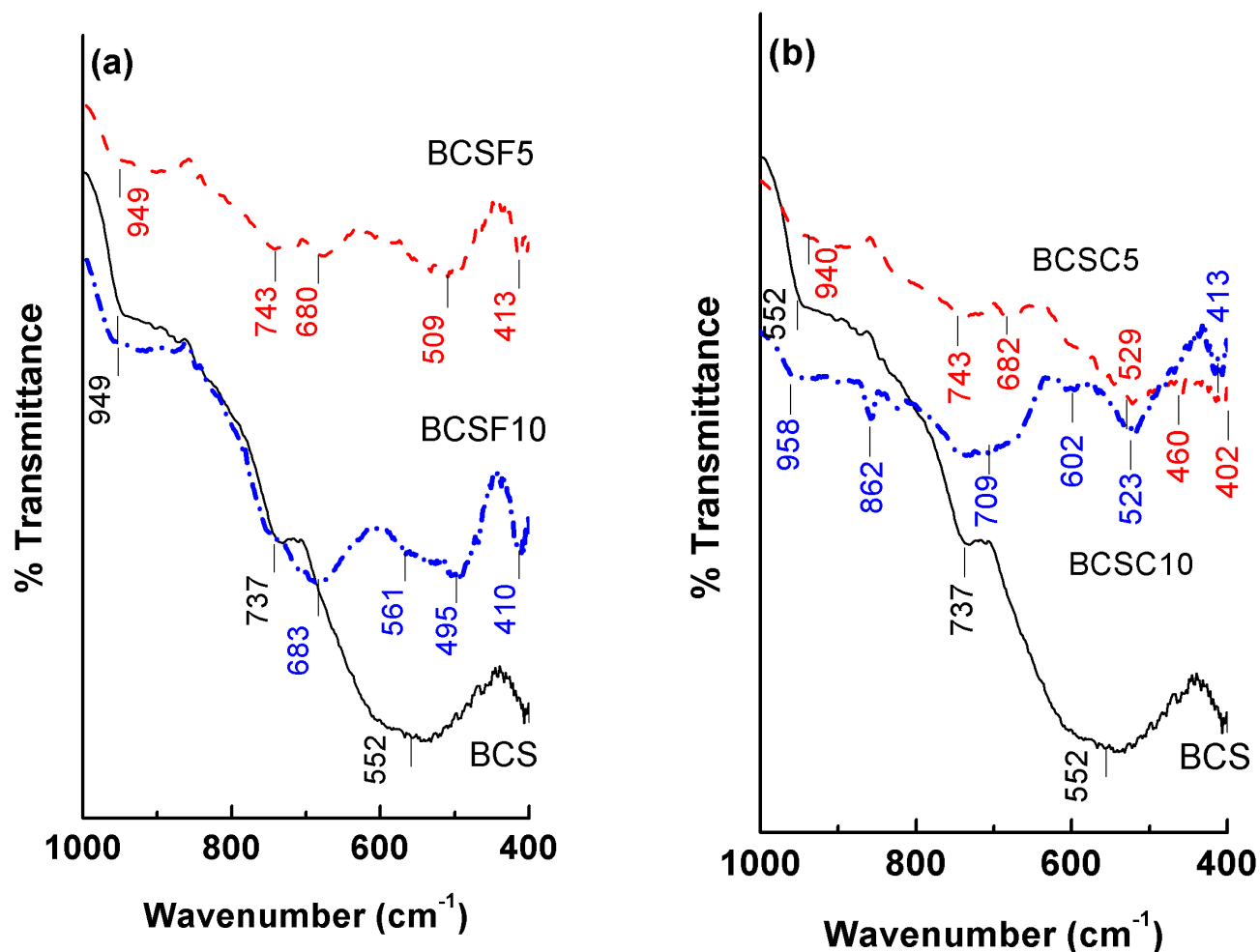


Figure S4. Room temperature FTIR in the region 1000- 400 cm^{-1} of (a) $\text{BaCe}_{0.9}\text{Sm}_{0.1}\text{O}_{3-\delta}$ (BCS), $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Fe}_{0.05}\text{O}_{3-\delta}$ (BCSF5), $\text{BaCe}_{0.8}\text{Sm}_{0.1}\text{Fe}_{0.1}\text{O}_{3-\delta}$ (BCSF10) and (b) $\text{BaCe}_{0.9}\text{Sm}_{0.1}\text{O}_{3-\delta}$ (BCS), $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Co}_{0.05}\text{O}_{3-\delta}$ (BCSC5), $\text{BaCe}_{0.8}\text{Sm}_{0.1}\text{Co}_{0.1}\text{O}_{3-\delta}$ (BCSC10) sintered powders at 1400 $^{\circ}\text{C}/8\text{h}$.

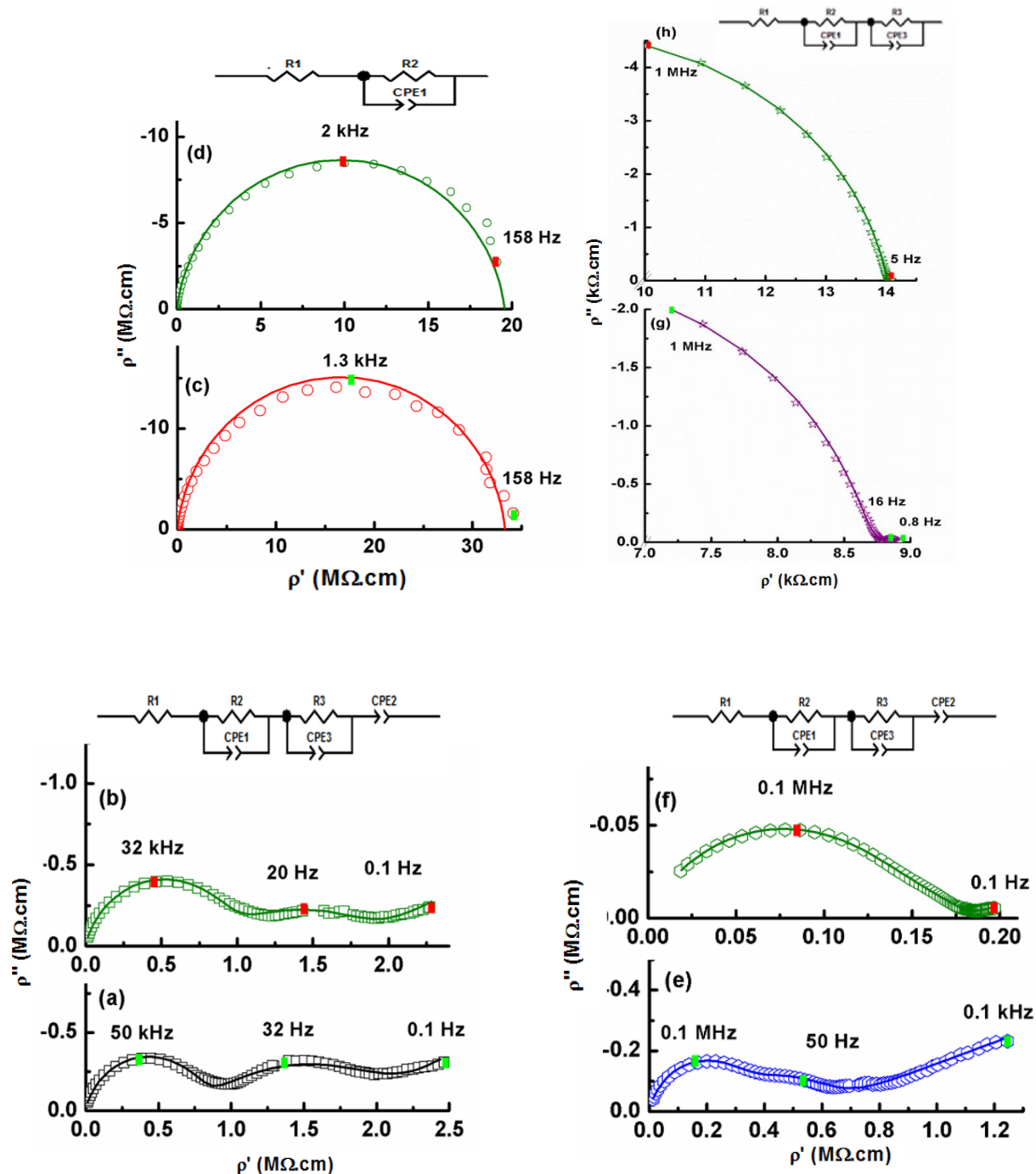


Figure S5. Impedance spectra of the 1400 °C sintered pellets that have the composition of (a,b) $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Fe}_{0.05}\text{O}_{3-\delta}$ (BCSF5), (c,d) $\text{BaCe}_{0.8}\text{Sm}_{0.1}\text{Fe}_{0.1}\text{O}_{3-\delta}$ (BCSF10), (e,f) $\text{BaCe}_{0.85}\text{Sm}_{0.1}\text{Co}_{0.05}\text{O}_{3-\delta}$ (BCSC5), and (g,h) $\text{BaCe}_{0.8}\text{Sm}_{0.1}\text{Co}_{0.1}\text{O}_{3-\delta}$ (BCSC10) measured at 90 °C in air, and $\text{H}_2 + 3\%\text{H}_2\text{O}$, respectively. The solid line represents the best fit from applying the corresponding equivalent circuit. All the plots were normalized to both the area and the thickness.