Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Controlling Surface Cation Segregation in Nanostructured Double Perovskite $GdBaCo_2O_{5+\delta}$ Electrode for Solid Oxide Fuel Cells

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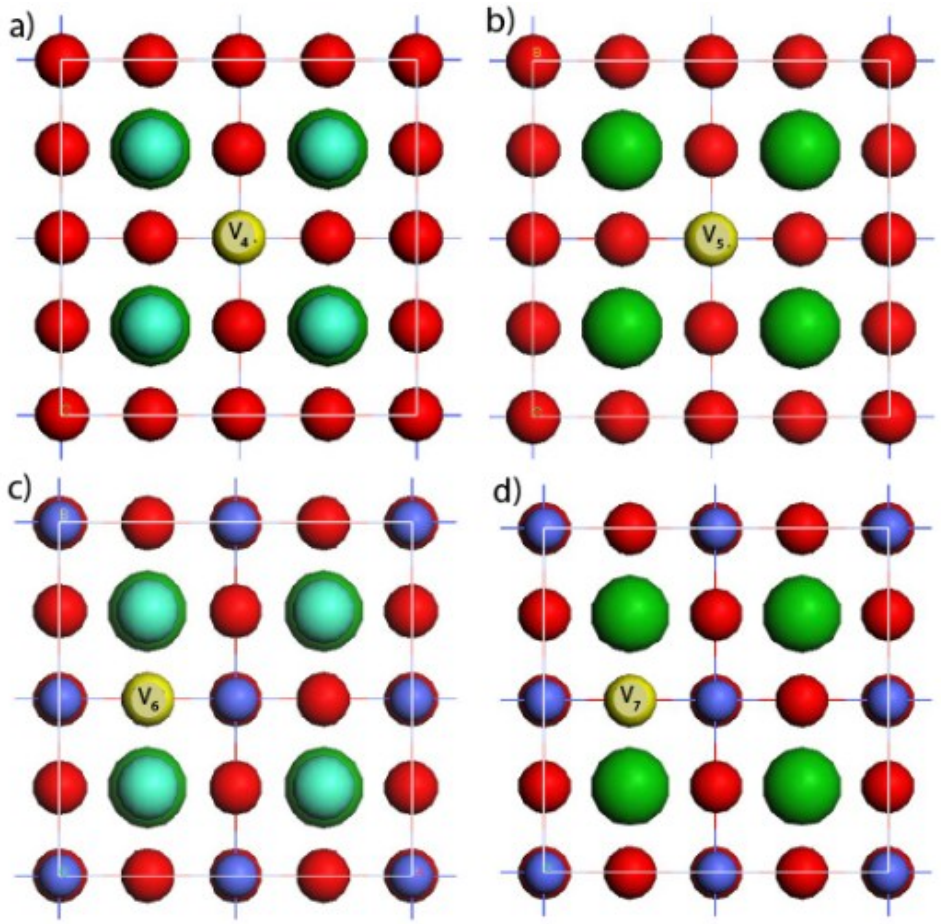

Figure S1 : Top view of a) Gd/Co, b) Ba/Co, c) Co/Gd, and d) Co/Ba terminal surfaces of GBCO lattice structure along (001) direction denoted as (cation present at surface / cation present at sub-surface). Gd, Ba, Co and O atoms are represented as sky blue, green, dark blue and red color respectively

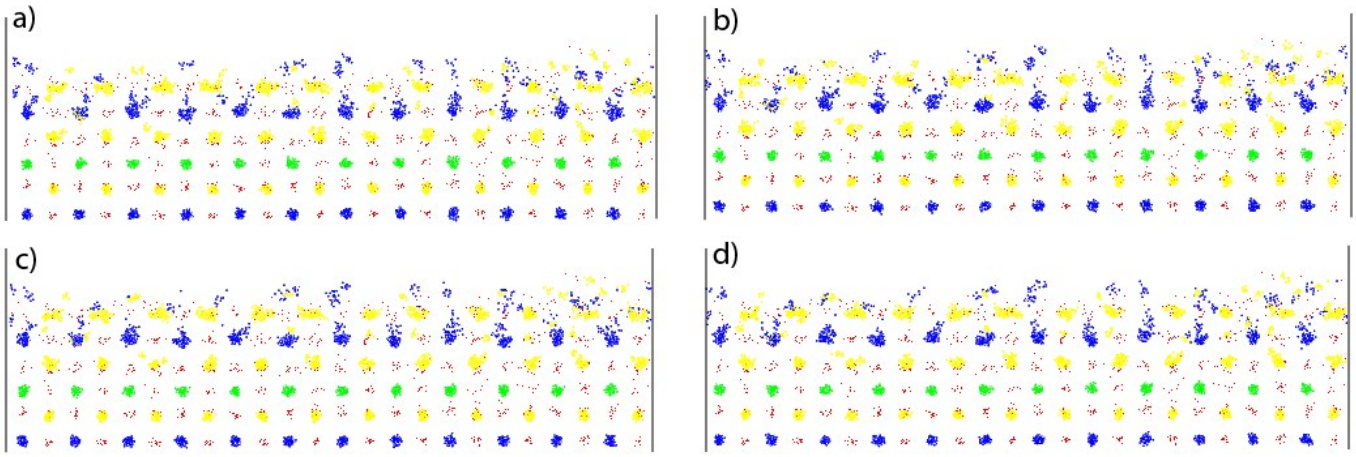

Figure S2: (a)-(d) Snapshots of the cation density profile of Co/Ba terminal surface of GBCO structure at the interval of every 10ps. Gd, Ba, Co and O atoms are represented as green, blue, yellow and red color respectively.

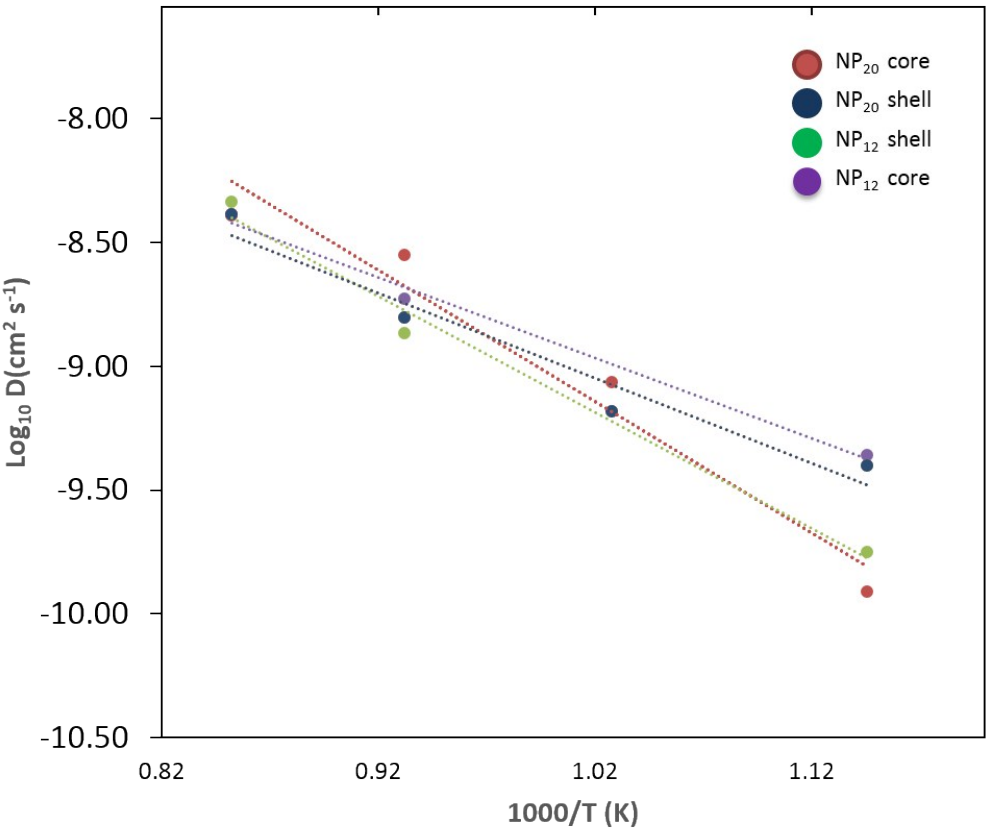

Figure S3: Arrhenius plot of core and shell diffusivity value for NP_{20} and NP_{12} nanoparticle for temperature range of 873 K-1173K

Table S1: Buckingham potential parameters

Interaction	**A_{ij} /eV**	**ρ_{ij} /Å**	**C_{ij} /eV Å**
Gd^{+3}-O^{-2}	1458.38	0.3522	0.0
Ba^{+2}-O^{-2}	1214.39	0.3537	0.00
Co^{+3}-O^{-2}	1329.82	0.3087	0.00
O^{-2}- O^{-2}	22764.3	0.149	43.00