Ab initio study of diffusivity and ionic conductivity of Ln$_2$NiO$_{4+\delta}$ (Ln=La, Nd, Pr) mixed conductor

Songye Yang$^1$, Guangchen Liu$^1$, Yueh-Lin Lee$^2$ Yu Zhong$^1$

$^1$Department of Mechanical and Material Engineering, Worcester Polytechnic Institute, 100 Institute Rd, Worcester, MA, 01609, USA

$^2$National Energy Technology Laboratory, 626 Cochran's Mill Road, P.O. Box 10940, Pittsburgh, Pennsylvania 15236-0940, USA

Introduction

SOFC: Solid oxide fuel cell
SOEC: Solid oxide electrolyzer cell

Vacancy formation energy (Ln$_2$NiO$_{4+\delta}$)

NEB calculations of Ln$_2$NiO$_{4+\delta}$

Objective of the work

Equation of state of Ln$_2$NiO$_4$ (Ln=La, Nd, Pr)

Temperature-dependent properties-Ln$_2$NiO$_{4+\delta}$

Comparison with exp:

Volume thermal expansion of Ln$_2$NiO$_4$ (Ln=La, Nd, Pr)

Comparison between different A-site elements

Conclusions

Electronic density of state (NNO)

Energy barrier of different paths

Selected diffusion paths

Electronic density of state (NNO)

Conclusions

Electronic density of state (NNO)

Conclusions

Electronic density of state (NNO)

Conclusions

Electronic density of state (NNO)

Conclusions

Electronic density of state (NNO)

Conclusions