First principles modeling of oxygen vacancy formation and mobility in (Ba,Sr)(Co,Fe)O₃₋ₓ perovskites

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Ba₁₋ₓSrₓCo₁₋ₓFeₓO₃₋ₓ perovskites: high concentration and mobility of Vₒ⁻

BSCF permeation membranes
• high D (Z.P. Shao (2000))

test as SOFC cathode
• high k (Z.P. Shao, S.M. Haile (2004))

mechanistic interpretation:
L. Wang, R. Merkle, J. Maier

Computational details

Electronic structure

Oxygen vacancy formation

Summary

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Vacancy formation energy Eᵥ, migration barrier Eₐ, and structural parameters of oxygen migration.

* spin projected density of states (DOS) for Ba₀.₉₁Sr₀.₀₉Co₀.₈₁Fe₀.₁₉O₃₋ₓ

Oxygen vacancy migration

Transition state:
• density map in (110) plane for Ba₀.₉₁Sr₀.₀₉Co₀.₈₁Fe₀.₁₉O₃₋ₓ
• "It's a triangle" and transition state relative to the ideal structure

Geometric factors: dₐ compared to BSCF
(cf. SrIr, SrBa and BaIr barriers for BSCF)

Electrical factors: vacancy formation energy (cf. SrIr barriers for BSCF, SCF, Bsf)

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