Strain Effect on Photocatalytic Oxygen Evolution Activity in Sr_3NF_3 Mixed Anion Perovskite Using First-principles Density Functional Theory (DFT)

Supplementary Information

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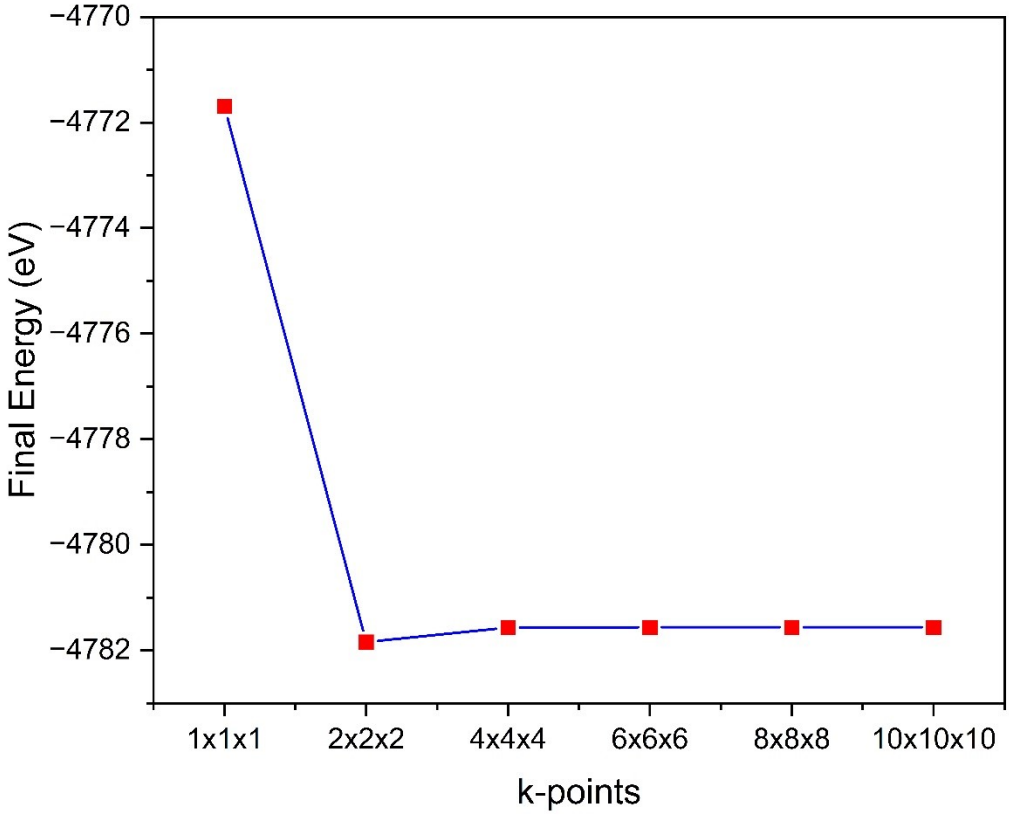

Figure S1: Convergence of total energy with respect to Monkhorst–Pack k-point mesh for Sr_3NF_3 calculated using the GGA-PBE functional.

Table S1: Comparison of experimental bandgaps (E_g^{Exp}) with theoretical values calculated using PBE (E_g^{PBE}) and HSE06 (E_g^{HSE06}) functionals for various perovskite materials[1]

Material	**E_g^{Exp} (eV)**	**E_g^{HSE06} (eV)**	**E_g^{PBE} (eV)**
$CsPbCl_3$	3.09	3.23	2.32
$CsSnI_3$	1.23	1.15	0.95
$CsGeBr_3$	2.15	1.97	1.35
$CsGeI_3$	1.67	1.61	1.12
$MAGeBr_3$	2.55	2.5	1.27

MA = $CH_3NH_3^+$

Table S2: Comparison of visible-light absorption coefficients of Sr_3NF_3 and representative photocatalysts reported in the literature.

Material	**Absorption coefficient (cm^{-1})**	**Wavelength (nm)**	**Reference**
$BiVO_4$	3×10^4	400	[2]
g-C_3N_4	~10^4	400-500	[3]
$SrTaO_2N$	3×10^4	320	[4]
Sr_3NF_3	3.7×10^4	320	This work

The reported absorption coefficients correspond to representative values in the visible region reported in the literature. Although the exact wavelength ranges differ slightly among materials, the comparison demonstrates that Sr_3NF_3 exhibits absorption coefficients comparable to established OER photocatalysts.

References:

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