From models to mechanisms: defects and charge trapping in amorphous silicon nitride

Hückmann, L.

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From Models to Mechanisms: Defects and Charge Trapping in Amorphous Silicon Nitride

PROEFSCHRIFT

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Promotor

Dr. J. Meyer

Co-promotor

Dr. J. P. Cottom

Promotiecommissie

Prof. dr.	M. Ubbink	
Prof. dr.	I. M. N. Groot	
Prof. dr.	M. I. J. Probert	(University of York)
Dr.	B. Weber	(ARCNL & Universiteit van Amsterdam)
Dr.	J. J. Geuchies	

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Contents

List of Abbreviations

Mathematical Symbols

x	scalar
$\boldsymbol{x}$	vectors
$\mathcal{N}$	normal distribution

Abbreviations

BO	Bayesian optimization
CBM	conduction band minimum
CTL	charge transition level
DOS	density of states
DFT	density functional theory
EPR	electron paramagnetic resonance
GGA	generalized gradient approximation
GPR	Gaussian process regression
GPW	Gaussian plane waves
HEG	homogeneous electron gas
IPR	inverse participation ratio
KS	Kohn-Sham
LDA	local density approximation
MAE	mean absolute error
MD	molecular dynamics
MQ	melt-quench
PBC	periodic boundary conditions

RDF	radial distribution function
VACF	velocity autocorrelation function
VBM	valence band maximum
VDOS	vibrational density of states

Physical Quantities

B	GPa	bulk modulus
E_{bg}	eV	band gap
E_{coh}	eV atom^{-1}	cohesive energy
E_{F}	eV	Fermi energy
E_{form}	eV	formation energy
ε_{r}		dielectric constant
$\Delta_{\mathrm{f}}H$	kJ mol^{-1}	heat of formation
μ	eV	chemical potential
μ_{s}	e	spin moment
ν	Hz	frequency
ρ	g cm^{-3}	mass density
ρ	$e\,a_0{}^{-3}$	electron density
q_{mul}	e	Mulliken charge

Kröger-Vink Defect Symbols

$\mathrm{X}_{\mathrm{S}}^{q}$	element X at site S in charge state q
H_{i}	hydrogen interstitials
N_{i}	nitrogen interstitials
V_{N}	nitrogen vacancy
O_{i}	oxygen interstitials
O_{N}	oxygen substitutions on nitrogen sites