

# Contents

<b>Acknowledgements</b>	<b>v</b>
<b>Abstract</b>	<b>vii</b>
<b>Zusammenfassung</b>	<b>ix</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Challenges in modern semiconductor device fabrication	1
1.2 Ab-initio simulations with VASP . . . . .	3
1.2.1 Static calculations . . . . .	4
1.2.2 Relaxations . . . . .	4
1.2.3 Molecular dynamics . . . . .	5
1.2.4 The nudged elastic band method . . . . .	6
1.3 Thermodynamics of crystal defects . . . . .	7
1.3.1 Formation energy . . . . .	8
1.3.2 Reaction enthalpy . . . . .	8
1.3.3 Binding energy . . . . .	9
1.3.4 Defect concentrations . . . . .	10
1.4 Some preliminary explanations . . . . .	11
1.4.1 Defect visualization . . . . .	12
1.4.2 Terminology . . . . .	13
1.4.3 Notation . . . . .	14
<b>2 Mixed phosphorus, arsenic and antimony clusters</b>	<b>17</b>
2.1 Cluster configurations . . . . .	18
2.1.1 Clusters of substitutional dopants . . . . .	19

2.1.2	Clusters with dopants and one vacancy . . . .	22
2.1.3	Clusters with dopants and one interstitial . . .	22
2.1.4	Clusters with dopants and two interstitials . .	24
2.2	Formation energies . . . . .	24
2.3	Binding energies . . . . .	28
2.4	Reaction enthalpies . . . . .	31
2.5	Conclusions . . . . .	32
<b>3</b>	<b>Fluorine clusters and diffusion</b>	<b>35</b>
3.1	Notation . . . . .	36
3.2	Cluster configurations . . . . .	36
3.3	Formation and binding energies . . . . .	38
3.4	Cluster concentrations . . . . .	40
3.5	The dominant mobile defect . . . . .	44
3.6	Conclusions . . . . .	46
<b>4</b>	<b>Arsenic diffusion in strained silicon</b>	<b>49</b>
4.1	Poisson ratio of silicon . . . . .	50
4.2	Mobile defects . . . . .	53
4.2.1	Configurations . . . . .	53
4.2.2	Formation energies . . . . .	54
4.2.3	Diffusion mechanism of AsV . . . . .	58
4.3	AsV diffusion in strained silicon . . . . .	61
4.4	Conclusions . . . . .	65
<b>5</b>	<b>Conclusion and outlook</b>	<b>67</b>
5.1	The diffusion concept . . . . .	67
5.2	Future work . . . . .	69
<b>A</b>	<b>Complementary investigations</b>	<b>71</b>
A.1	Lattice constant of crystalline silicon . . . . .	71
A.2	Accuracy evaluation of the simulation results . . . . .	72
A.3	Determination of minimum energy configurations . . .	77
A.4	Energy correction for charged defects . . . . .	77
A.4.1	The correction method . . . . .	78
A.4.2	Applications . . . . .	80
	<b>Curriculum vitae</b>	<b>91</b>