

Colin Howard

Measuring, Interpreting  
and Translating Electron  
Quasiparticle – Phonon  
Interactions on the Surfaces  
of the Topological Insulators  
Bismuth Selenide  
and Bismuth Telluride

Doctoral Thesis accepted by Boston University, Boston,  
Massachusetts, USA

 Springer

# Contents

<b>1 Introduction</b> .....	1
References .....	5
<b>2 Properties of <math>\text{Bi}_2\text{Se}_3</math> and <math>\text{Bi}_2\text{Te}_3</math></b> .....	7
2.1 Crystal Structure .....	7
2.2 Bulk Vibrational Structure .....	9
2.3 Electronic Structure .....	11
References .....	14
<b>3 Helium Atom-Surface Scattering (HASS)</b> .....	15
3.1 The Benefits of HASS .....	15
3.2 The Surface Interaction Potential .....	16
3.3 The Kinematics of HASS .....	18
3.3.1 Elastic Scattering .....	18
3.3.2 Inelastic Scattering and Time-of-Flight Technique .....	19
References .....	22
<b>4 Experimental Apparatus and Technique</b> .....	23
4.1 Surface Laboratory Facilities .....	23
4.2 Source Chamber .....	23
4.3 Target Chamber .....	26
4.3.1 Production and Monitoring of UHV .....	27
4.3.2 Sample Manipulator .....	27
4.3.3 Sample Cleaver .....	28
4.3.4 Helium Detector .....	29
References .....	31
<b>5 Pseudocharge Phonon Model</b> .....	33
5.1 Fundamentals of the Model .....	33
5.2 Adiabatic Approximation, Ionic Self-Terms, and PC Self-Terms .....	34
5.3 Bulk Parameters .....	36
5.4 Surface Parameters .....	41
References .....	42

<b>6</b>	<b>HASS Results from the Surface of <math>\text{Bi}_2\text{Se}_3</math> and <math>\text{Bi}_2\text{Te}_3</math></b> .....	43
6.1	Elastic and Inelastic Scattering Results .....	43
6.2	Calculation of EPC Parameter in the Random Phase Approximation .....	48
	References .....	53
<b>7</b>	<b>Translating Between Electron and Phonon Perspectives</b> .....	55
7.1	Motivation .....	55
7.2	DFQ Self-Energy Formalism .....	56
7.3	Computational Results .....	58
7.4	Additional Supporting Results .....	62
	References .....	64
<b>8</b>	<b>Conclusion and Future Directions</b> .....	65
8.1	Summary .....	65
8.2	Future Work .....	66
	References .....	70
<b>A</b>	<b>Supplemental Material for Electron Self-Energy Analysis</b> .....	71
A.1	Electron Green's Function .....	71
A.2	Bosonic Sums .....	77
<b>B</b>	<b>Numerical Evaluation of the DFQ Self-Energy</b> .....	81
B.1	Hole Term .....	82
B.1.1	Above Dirac Point .....	82
B.1.2	Below Dirac Point .....	86
B.2	Particle Term .....	86
B.2.1	Above Dirac Point .....	86
B.2.2	Below Dirac Point .....	87
B.3	Interband Transitions .....	88