1 Introduction to Superconductivity in Alkali-Doped Fullerides
   1.1 Superconductivity in Alkali-Doped Fullerides
   1.1.1 Historical Background
   1.1.2 Properties of Alkali-Doped Fullerides Revealed by Experiments
   1.1.3 Electronic Structure and Electronic Correlations
   1.1.4 Electron-Phonon Interactions and Phonon Frequencies
   1.1.5 On Applicability of Conventional Mechanism
   1.1.6 Unconventional Mechanisms
   1.2 Aim of the Thesis
   1.3 Outline of the Thesis
References

2 Methods: Ab Initio Downfolding and Model-Calculation Techniques
   2.1 Multi-energy-scale Ab Initio Scheme for Correlated Electrons (MACE)
   2.1.1 General Framework
   2.1.2 Low-Energy Effective Hamiltonian
   2.2 Ab Initio Downfolding for Electron-Phonon Coupled Systems
   2.2.1 Density Functional Theory
   2.2.2 Maximally Localized Wannier Function
   2.2.3 Constrained Random Phase Approximation
   2.2.4 Density-Functional Perturbation Theory
   2.2.5 Constrained Density-Functional Perturbation Theory
   2.3 Analysis of Low-Energy Hamiltonian
   2.3.1 Dynamical Mean-Field Theory
   2.3.2 Extended Dynamical Mean-Field Theory
   2.3.3 Impurity Solver: Continuous-Time Quantum Monte Carlo Method
### 2.3.4 Simulation of Superconducting State Within Extend
DMFT .................................. 85

### 2.4 Combining Model Derivation and Model Analysis ............. 90
2.4.1 Interfaces ................................... 90
2.4.2 Overview of Whole Scheme .......................... 95

References ................................................. 98

### 3 Application of cDFPT to Alkali-Doped Fullerides ............... 101
3.1 Calculated Materials and Calculation Conditions ............... 101
3.2 cDFPT Results ...................................... 103
3.2.1 Partially Renormalized Phonon Frequencies .................. 103
3.2.2 Effective Onsite Interactions Mediated by Phonons .......... 104
3.2.3 Dynamical Structure of Onsite Interaction Including
Coulomb and Phonon Contributions Along Real
Frequency Axis ........................................... 106
3.3 Comparison Between Partially Renormalized and Fully
Renormalized Quantities .................................. 107
3.3.1 Difference in Frequencies ............................ 108
3.3.2 Difference in Phonon-Mediated Interactions ................ 109
3.4 Smallness of Electron-Phonon Vertex Correction
in Downfolding Procedure ................................ 113

References ................................................. 116

### 4 Analysis of Low-Energy Hamiltonians with Extended DMFT ...... 119
4.1 Input Parameters ..................................... 119
4.2 Frequency Dependence of Effective Onsite Interaction ....... 120
4.3 Phase Diagram ....................................... 121
4.3.1 Comparison Between Theory and Experiment ............... 121
4.3.2 Accuracy of Phase Boundaries ........................ 122
4.4 Metal-Insulator Transition ................................ 123
4.4.1 Physical Quantities at 40 K .......................... 123
4.4.2 Spectral Functions .................................. 126
4.5 Nature of Superconductivity ................................ 128
4.5.1 Gap Function ...................................... 128
4.5.2 Pairing Mechanism .................................. 129
4.5.3 Possible Explanations on Origin of Dome-Shaped $T_c$ ...... 131

References ................................................. 134

### 5 Concluding Remarks ....................................... 137
5.1 Summary of the Thesis .................................. 137
5.2 Future Issues ......................................... 138

References ................................................. 140

Curriculum Vitae ........................................... 141
Ab Initio Studies on Superconductivity in Alkali-Doped Fullerides
Nomura, Y.
2016, XX, 143 p. 27 illus., 18 illus. in color., Hardcover
ISBN: 978-981-10-1441-3