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Theoretical Study of Electron-Phonon Interactions in Isotopic Diamond Superlattice

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In Chapter 1, we introduce the backgrounds of this study. We explain phononics, electron-phonon interactions, isotope effects, and superlattice. Then, we introduce isotopic diamond superlattice (IDS) and related phenomenon. We summarize the objectives of this study at the end of this chapter.

In Chapter 2, we review the theoretical backgrounds used throughout this study. We start from the Born-Oppenheimer approximation and explain the density functional theory, the Wannier function, the density functional perturbation theory, the force constant model, the Allen-Heine-Cardona theory, the Wannier representation of electron-phonon interactions, and the concept of the quasiparticle self-consistent GW.

In Chapter 3, we show the results of phonon calculations in several isotopic diamond superlattices because phonon localizations due to isotope effects should be one key point causing the formation of quantum wells.

In Chapter 4, we introduce the details of our quasiparticle tight-binding model. We construct tight-binding model from the Wannier representation of electron-phonon interactions with some approximations. We apply the numerical method of the quasiparticle self-consistent GW to calculations for electron-phonon interactions.

In Chapter 5, we discuss the validity of our quasiparticle tight-binding model in comparison with first-principle calculations based on the density functional perturbation theory. We carry out computations of zero-point renormalizations in isotopically pure ^{12}C diamond by using both our quasiparticle tight-binding model and first-principle calculations.

In Chapter 6, we show and discuss electronic states including zero-point renormalizations obtained by our quasiparticle tight-binding model in virtual ^{6}C/^{24}C [001] IDS. Since the difference of the bulk zero-point renormalizations between virtual ^{6}C and ^{24}C diamonds becomes larger than that between real ^{12}C and ^{13}C diamond, virtual ^{6}C/^{24}C [001] IDS is regarded as an ideal IDS forming quantum wells.

In Chapter 7, we show the numerical results obtained by our quasiparticle tight-binding model in real $^{12}C/^{13}C$ [001] IDS. We report the thickness of each isotopic diamond layer where the formation of quantum wells occurs.

In Chapter 8, we make conclusions and provide future works about this work.