別紙１－１

論文審査の結果の要旨および担当者

報告番号	※　甲　第　　号

氏　　名　西　本　佳　央

論　文　題　目　Method Development for Approximate Density Functional Theory and Applications to Complex Molecular Systems

（近似的密度汎関数法のための手法開発と複雑な分子系への応用）

論文審査担当者

主　査　名古屋大学トランスフォーマティブ生命分子研究所
教　授　Ph.D.　IRLE Stephan

委　員　名古屋大学大学院理学研究科　教　授　理学博士　阿波賀　邦夫

委　員　名古屋大学トランスフォーマティブ生命分子研究所
特任准教授　博士（工学）横川　大輔

別紙１－２

論 文 審 査 の 結 果 の 要 旨

From the very beginning the candidate was involved in the development and application of the density-functional tight-binding (DFTB) method, which is an approximation to the traditional density functional theory (DFT) quantum chemical method. DFT is widely used by theoreticians and experimentalists alike to compute chemical and physical properties and reaction energy profiles for systems containing up to several 100 atoms. However, the bottleneck of traditional DFT methods is the relatively long computer time required for systems containing more than a few hundred atoms: a) molecular dynamics simulations are limited to only 10 to 100 picoseconds, and b) vibrational and optical spectra can only be computed for systems containing about to about 100 atoms, even when using DFT methods that scale linearly with system size and are optimized to run on massively parallel computers such as the K supercomputer in Kobe. In our group we try to reduce the computer time requirements of traditional DFT by further developing the DFTB method, being roughly 3-5 orders of magnitudes faster. Nishimoto-san was one of the driving forces in our group towards this development, and it is documented in his 9 peer-reviewed papers, 4 of which are first-author papers.

Mr. Nishimoto's thesis presents three chapters, the first two of which are related to the DFTB development, while the third is an application of traditional DFT to follow structural changes induced in polyoxymetalate clusters upon super-reduction by a large number of excess electrons. In the first chapter, Nishimoto-san combined the well-known, linearly-scaling "Fragment Molecular Orbital" (FMO) method with DFTB and created the new, extremely fast and linearly scaling FMO-DFTB method, which runs well on parallel computer platforms and can be applied to biosystems as well as materials science problems. Using this method, it was possible for instance to optimize the geometry of a fullerite slab consisting of more than 1,000,000 atoms, which is one of the records in the literature for quantum chemical methods. In the second chapter, the candidate extended the analytical second order geometrical energy derivatives such that vibrational infrared (IR) and Raman spectra can be simulated even for systems with small or zero HOMO-LUMO gaps, including radicals and metallic systems. In the third chapter, Mr. Nishimoto used a combination of DFT with molecular dynamics to identify the origin of metal-metal bonds formed during superreduction in cathode-active polyoxymetalate clusters, studied experimentally in the Awaga group in our Department.

Mr. Nishimoto defended his PhD thesis well using the English language throughout his presentation, and was able to address the questions of the present faculty members well, also in the English language. The present faculty members as well we as the reviewers agree with me that the candidate deserves to obtain the Doctoral Degree.