別紙１－１

論文審査の結果の要旨および担当者

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氏　　名　Arifin

論　文　題　目　Theoretical investigation of complex molecular systems:
Structures, chemical reactions and spectroscopy
（複雑分子系の理論的研究：構造、化学反応、分光測定の理解に向けて）

論文審査担当者

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論 文 審 査 の 結 果 の 要 旨

Arifin came to us as a G30 PhD student from the quantum chemistry group of Professor Muhamad Martoprawiro at the ITB Bandung in Indonesia, one of that country's most prestigious academic research institutions. When the candidate moved to our lab to conduct his PhD studies in our Quantum Chemistry Laboratory, he already had the necessary skills to perform quantum chemical calculations on molecules in their ground electronic states in the gas phase. During his studies in our lab he learned to search and find efficiently transition state structures of chemical reactions, and to perform quantum chemical calculations in solution. In addition, he learned the formalism and application of the density-functional tight-binding (DFTB) method, which is currently developed in our lab. He applied this method in the theoretical simulation of vibrational spectra of nanometer-sized moleculer systems, as will be described below.

In research topic i), the candidate studied the importance of short and long-range solvation effects on the stability of the glucose anomers by the combination of quantum mechanics (QM) and statistical mechanics, namely the reference interaction site model self-consistent field spatial electron density distribution (RISM-SCF-SEDD). The preferences of α- and β-glucose in gas phase and various solvents were well reproduced. In the case of strongly interacting solvents, such as DMSO and ionic liquids, the solvation structures around the anomeric sites clearly show that the short-range interactions between solute and solvents determine the stability of one anomer over the other. On the other hand, long-range interactions are dominant in the case of solvation in acetone, acetonitrile, and H_2O.

In research topic ii), the candidate studied the chemical transformation of glucose to hydroxylmethylfurfural (HMF), a compound of great industrial importance. To convert otherwise unusuable biomass into such a value-added chemical compound, ionic liquids have proven to be useful to lower the energy requirement for this transformation reaction. Mr. Arifin found that the chemical reaction mechanism pathway differs from water and ionic liquid solvents, in the former, a cyclic reaction mechanism is energetically favorable, whereas in the latter, an open-chain mechanism dominates. Knowledge of dominant reaction mechanism will help to optimize the transformation reaction on industrial scale.

In research topic iii), the candidate found that the dependence of the low-frequency Raman-active breathing modes of carbon nanomaterials on the size of the molecular systems can be extrapolated using a simple equation involving the dimensionality of the material, namely 1D for polyynes, 2D for graphene nanoribbons and flakes, and 3D for nanodiamonds. This surprising fact had not been reported before.

In the thesis defense presentation on February 23, the candidate explained his research results well and was able to explain detailed questions to the satisfaction of the reviewers.