別記様式第４号

論文博士用

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平成 11 年 3月 19 日

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論文審査及び学力の確認の結果報告書

このことについて、下記の結果を得ましたので報告いたします。

記

学位申請者	相田正之	報告番号	第 121 号
申請学位	博士（工学）	専攻名	機能材料工学専攻
論文題目	STUDIES ON ELECTRONIC STATES OF POLYMERS IN X-RAY PHOTOELECTRON SPECTROSCOPY BY MOLECULAR ORBITAL METHODS USING THE MODEL MOLECULES （分子軌道(MO)法によるポリマーのXPSスペクトル解析に関する研究）		
公開審査会の日	平成 10 年 8 月 18 日		
論文審査の期間	平成 10年 7月 23日～平成 11年 3月 18日	論文審査の結果	合格
学力の確認の日	平成 10 年 8 月 18 日	学力の確認の結果	合格

論文内容の要旨

The submitted thesis deals with theoretical and computational interpretation of X-ray photoelectron spectra of polymers. The computations are based on semiempirical and non-empirical quantum-chemical calculations combined either with Koopmans' theorem or with the Slater transition state concept. The studied polymers are for example: polyvinylalcohol, polyvinylchloride, polyvinylacetate, etc. They are simulated either by a crystal model with one-dimensional periodicity, or by small oligomers like dimers or trimers. The employed quantum-chemical treatments range from the PM3, AM1, and HAM/3 semiempirical methods, through ab initio Hartree-Fock treatments, to ab initio density-functional-theory approaches, and various quantum-chemical software packages have been applied. The theoretical analysis aims at an acceptable reproduction of the energy position and intensity of the observed spectral peaks, and adjusts the computational outputs to this goal. In addition to the reproduction, also a deeper insight into the observed spectra or even their predictions are possible.

審査結果の要旨

The submitted thesis was prepared during research works at the Mitsubishi Paper Mills Tsukuba Res. Lab. The research results have been published in six original papers published in Curr. Cont. covered journals (J. Phys. & Chem. Solids, Polymer. J., Bull. Chem. Soc. Jpn.). The thesis deals with a significant problem and uses up-to-date computational methods. As the results have been published over a period of five years, the computational tools have gradually been adjusted to the fast development of computational chemistry. The results achieved well correspond to the research standard of other groups in the field, and in fact a part of them is based on an international co-operation. The developed approach offers a reasonably reliable tool for reproduction and interpretation of the observed X-ray photoelectron spectra of polymers. It advances in both key issues - computations of the energy position and peak intensity, and offers some deeper insights into the physical nature of the observed phenomena. The level and extent of the presented results represent a solid ground for the PhD-degree award.

審査委員

スラニナ 印　大澤映二 印　遠藤一央 印

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（注）　論文審査の結果及び学力の確認の結果は「合格」又は「不合格」の評語で記入すること。