論文 / 著書情報
Article / Book Information

題目(和文)	CH3Fをドープした固体パラ水素の局所的な構造に対する中赤外高分解能分光研究
Title(English)	High resolution infrared spectroscopic studies for the local structure of para-hydrogen crystal around dopant CH3F
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Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

（博士課程）
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論 文 要 旨

THESIS SUMMARY

専攻： Department of	物性物理学　専攻	申請学位（専攻分野）： Academic Degree Requested	博士　（　理学　） Doctor of
学生氏名： Student's Name	川﨑　博之	指導教員（主）： Academic Advisor(main)	金森　英人　准教授
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

Solid *para*-H_2 is well known as a prototypical quantum solid. There has been considerable previous experimental and theoretical research. However, the characters of the local structure of *p*-H_2 crystal around dopant have not been cleared yet. This research surveyed mainly four physical subjects related to the local structure of solid *p*-H_2 around dopant molecule. The first subject is about the nuclear spin conversion rate of *o*-H_2 molecule in solid *p*-H_2. The temporal behaviors of the absorption spectrum of CH_3F-(*o*-H_2)$_n$ were observed. The spectral change is caused by the nuclear spin conversion of *o*-H_2 molecules in the first nearest neighbor site of CH_3F. The self-conversion rate and the catalyzed-conversion rate were estimated by fitting analysis. The decay time of the catalyzed-conversion was estimated to be 24.4(8) hours. This is the first time to estimate the catalyzed-conversion rate between one *o*-H_2 and one dopant molecule. From this research, we found that the catalyzed-conversion rate of *o*-H_2 by CH_3F is faster than the self-conversion rate, but the difference between them are not so large. The effect of CH_3F to the nuclear spin conversion of *o*-H_2 is not only to do the catalyzed-conversion, but also to accelerate the self-conversion of *o*-H_2 since CH_3F makes *o*-H_2 molecules come close to it. Thus, the effects of the dopant molecules to the nuclear spin conversion of *o*-H_2 should be treated from some points of view. This research could contribute not only to the knowledge of the system of CH_3F in solid *p*-H_2 but also the development of the detailed physical implications of nuclear spin conversion of *o*-H_2 with the dopant in solid *p*-H_2. The second subject is about the origin of unknown peaks. New satellite series were found to the lower energy side of each main peak of the ν_3 band of CH_3F embedded in a *p*-H_2 crystal. All the peaks showed a common red shouldered line profile, which corresponds to partly resolved transitions of *ortho*- and *para*- CH_3F. Some experimental results may suggest that these satellite series originate from a family of CH_3F clusters involving *o*-H_2 in second nearest neighbor sites. A model function assuming this idea was used to resolve the observed spectrum into each Lorentzian component, and then the detailed features of these series were studied. The peak intervals in the series are not as equally spaced as the main series, but there is a strong resemblance to the satellite series. We proposed that the effect of *o*-H_2 molecules in the second nearest neighbor site of CH_3F could not be ignored. The third subject is about the alignment of the dopant molecule. The polarization dependence of the ν_3 vibrational transition of CH_3F, whose rotational motion is hindered in *p*-H_2 crystal, was observed. The experimental results were well explained by a simple six-way vacancy model and the alignment angle in the crystal is determined. The CH_3F is not aligned along the *c*-axis but tilted to 64° from the *c*-axis. This is the first time to estimate the alignment of dopant molecule in solid *p*-H_2 by experimentally. The method to estimate the alignment of the dopant can be used for other dopant molecules. This research could contribute to some studies, like which use the orientation of dopant molecules. The fourth subject is about the structural changes of CH_3F-(*o*-H_2)$_n$ by the pumping lasers. By using two QC lasers, the processes of the structural change by the pumping beam were observed at the first time. In order to estimate each rate for the structural change of each cluster, these pump-probe experimental results were analyzed by using some model functions. The fitting results showed that the local thermal energy of the *p*-H_2 crystal around CH_3F increases and the resonance frequency of the CH_3F in the cluster is shifted. This research could contribute to understanding the mechanism of the thermal relaxation in solid *p*-H_2 around dopant. In addition, some unknown peaks (e.g. the *d* series and *n* = 3' peak) have been surveyed. The characters and the origins for them were proposed. Some theoretical supports are quite important for the determination of the origins of these peaks. From this research, some characters of solid *p*-H_2 to the dopant molecule were cleared. Furthermore, this research developed the knowledges about the interaction between *o*-H_2 molecules and CH_3F. The characters of the local structure of solid *p*-H_2 revealed in this research are not only for dopant CH_3F. These achievements can contribute to the studies for other dopants in solid *p*-H_2 and also the studies for the characters of solid *p*-H_2 itself.

備考 ： 論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。
Note : Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1copy of 800 Words (English).