A unified understanding of the chemical bond in hydrogen storage materials by electron density distributions and its application to quantum materials design

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【Outline of survey】

Knowledge of spatial electron density distribution, $\rho(r)$, is so fundamental for the understanding of the nature of the chemical bond between atoms in every material. Recently, a universal relation between electron density minima, ρ_{min} ,and atomic or ionic radii, r_{min} , has been discovered by us from the first principles calculations of electronic structures over 150 species, including gasses, water and solids. It is expressed as, $\log [\rho_{min}/Z^3] = -5.29 \log [1.01 + 0.285x\ 2(Z/n) r_{min}]$, where Z is the atomic number of element and n is a principal quantum number. On the basis of this discovery, we aim to break new ground for hydrogen materials science. To this aim, electronic structures of diatomic molecules and simple binary hydrides are calculated by the first principles calculation methods, and then a basic equation for the binding energies between hydrogen and metals (or non-metals) in them will be formulated using two variables, ρ_{min}/Z^3 and $2(Z/n) r_{min}$. The application of this equation to a variety of hydrides may allow us to get a common rule, characteristic of the hydrogen chemical bonds in many hydrides. Then, a solid ground of hydrogen materials science could be built up by combining these calculations with the Raman spectroscopic experiments to account for the atomic vibration modes around hydrogen. An electron-design map as well as a new platform for materials design will be constructed on this ground and used for the development of noble hydrogen storage materials.

【Expected results】

One of the expected productions is to obtain simple understanding and expression for the factors to control the cohesive mechanism between hydrogen and metals (or non-metals) in hydrides. Quantitative hydrogen-metal bond strengths will be obtained for the first time through this study. Any qualitative expressions of chemical bonds such as covalent bond or ionic bond are no longer needed to specify the chemical bond in the hydrides. Second expected production is to collect the Raman spectroscopic data experimentally for the further understanding of hydrides in view of hydrogen vibration modes. Third one is to construct an electron-design map and a new platform for materials design by combining these calculations and experiments. A series of the present approaches will lead to the effective development of new hydrogen storage materials.

【References by the principal researcher】

M. Yoshino, M. Morinaga et al., " A Universal Relation between Electron Density Minima and Ionic Radii in Ceramics ", *Materials Transactions*, 45 (2004), 1968-1972.

【Term of project】 FY 2005 - 2009	**【Budget allocation】** 89,500,000 Yen

【Homepage address】 http://sigma.numse.nagoya-u.ac.jp/