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How to Predict New Nano-structured Materials with Confidence? -Theoretical Study on Task Specific Ionic Liquid for Metal Extraction from Garbage Caused by Tsunami-

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In the 50 years of the history of DFT proposed by Professor Walter Kohn in 1964, applying this formulation, a number of ab initio calculations have been performed to explain experimental observations and to predict new materials from atomic and electronic levels. Unfortunately, recent trend is to increse number of atoms to treat complex systems and to include parameters such as U for band-gap fitting or to modify Exc for van der Waals interaction, and shifting to phenomonology. By these methods, we can only explain experimental data, but not have good confidence to design new materials. In the talk, I will introduce several new methods which certifies our ab initio calculations with confidence; (1) initial atomic configurations desining with mathematicians based on symmetry consideration, (2) checking necessary conditions such as virial theorem and cusp condition, and (3) checking dynamical stability by phonon calculation.
After 5 years from the big tsunami attaked Tohoku area in Japan, still there remain a large amount of garvages. They have been collected to limited areas and classified as stones, steels, woods, etc., and among them there are a large amount of electronic circuit boards, which contain expensive metals should be reused. We have been trying to extract such metals by using ionic liquid experimentally and theoretically. The ionic liquid is functionalized by attached ligands for extraction of specific metal element, and is called “task specific ionic liquids (TSIL)”. Since the properties of TSIL varies strongly as a function of temperature and not easy to understand experimentally, especially temperature dependence of viscosity and hydrophobicity are difficult. We have developed a new theoretical method based on molecular dynamics and hydrodynamics to determine theoretically the viscosity in TSIL, and successfully applied to compute for several TSIL Up to the present Rh has been the worst to be extracted efficiently from garvage in industry. We studied the properties of Rh and proposed a new TSIL, which atomic structure is shown on the right and is expected to be suitable for Rh extraction compared to existing industrial methods.

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