Higher Level of *ab initio* Computer Simulation for Materials Design – How to Perform Theoretical Design of Materials

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To understand the phenomena used in nanomaterials for energy conversion and fuel cell, it is necessary to apply *ab initio* computer simulation. Especially to design theoretically new nanomaterials for such applications, still fundamental problems should be studied carefully and developed to match to the requirement. However, the present status of the *ab initio* computer simulation based on the density functional theory generally used is not good enough, since it is a ground state theory and does not show any exchange-correlation functional. To be able to proceed more than the present level of the theory to understand the physical properties of nanomaterials and design them without experimental help, it is not sufficient to use commercialized *ab initio* software, and researchers should develop a software, which can be really applicable to predict new useful nanomaterials. In the talk, the speaker will introduce severe problems in the widely used *ab initio* software, and indicate better approach such as the time dependent density functional theory recently implemented in the TOhoku all electron Mixed Basis Orbitals *ab initio* approach, TOMBO, which can trace chemical reaction beyond the adiabatic approximation and is important in designing fuel cell materials. The speaker will also introduce some of the new developments of thermoelectric conversion, by the speaker and his research group, in TOMBO based on the 3^{rd} and 4^{th} derivative of the total energy, and Van der Waals interaction derived from dipolar polarization for hydrogen storage materials. The software TOMBO is available for researchers in materials design by computer simulation in Asia region (as a member of Asian Consortium on Computational Materials Science, ACCMS) provided that they work collaboratively with the research group.