

## Mathematics-Materials science Cooperation

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The major research direction at AIMR is to develop cooperation between mathematics and materials sciences to achieve revolutionary new concept of materials and their functionalization. In this talk, some examples of the collaboration between mathematics/theory and materials sciences are introduced.

The first example is the topics of atomic structure analysis of metallic glasses with collaboration of angstrom beam electron diffraction and computational homology. The new approach provides a general method for a clear description of short to mid range orders of amorphous materials beyond conventional two-body distribution functions. Next topics is on the recent results of nano-level structuring of water/aqueous solution obtained by the first-principles MD calculations as well as AFM observation. It will be shown that regular hydrogen bond(HB) chains or their rings play an important role of non-local molecular splitting of water causing significant influences on (electro-)chemical processes of water/aqueous solution. Final topics is on the competing wave-like or particle-like features of electron/hole transport in middle size molecules or long chain molecules bridging between electrodes. As wave-nature predominating cases, we will introduce theoretical prediction of large internal loop currents in fullerene, triangular graphene, certain kinds of CNT tori, and on a particle-nature predominating case, we show the Frank-Condon blockade of C<sub>60</sub> between nano-electrodes. Finally for the case of long helical polyacetylene, Poly(octyloxyphenylacetylene) POOPA, we can see a transition from the wave-like to particle like diffusion by analyses with time dependent wave-packet diffusion method. A unique feature, multi pass transport, characteristic of helical structures is found.

[1].Mitsutake M, Yano K, Tsukada M; in press, *J. Phys. Chem.2015* , DOI:10.1021

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### Education

1970 PhD, solid state physics (Theory) University of Tokyo  
1965 BSc, solid state physics (Theory) University of Tokyo

### Professional Experience

|   |           |
|---|-----------|
| Specially appointed Professor   |           |
| Administrative Director, at AIMR, Tohoku University,                                  | 2012-2015 |
| Professor, PI, at AIMR, Tohoku University   | 2008-2012 |
| Professor at Graduate School of Advanced<br>Science and Technology, Waseda University | 2004-2008 |
| Professor at Faculty of Science, University of Tokyo                                  | 1991-2004 |
| Associate Professor at Faculty of Sci., Univ. of Tokyo                                | 1982-1991 |
| Associate professor at Institute for Molecular Science                                | 1976-1982 |
| Research Associate at Faculty of Sci., Univ. Tokyo                                    | 1970-1982 |

### Fields of Research

Theory of SPM and nano-structures, modeling and computations

### Publications

1. Hamada I, Shimizu R, Ohsawa T, Iwaya K, Hashizume T, Tsukada M, Akagi K, Hitosugi T, Journal of the American Chemical Society, **136** 17201 (2014)
2. H.Tamura, Tsukada M, Ishii H, Kobayashi N, and Hirose K, Physical. Review. **B87**, 155305 (2013)
3. Tamura H, Tsukada M, McKenna, K.P, Shluger A.L, Ohkubo T, Hono K, Physical Review **B 86**, 195430 (2012)
4. Tsukada M, Masago A, Shimizu M, Journal of Physics, Condensed Matter, **24** 984002 (2012)
5. Araidai M, and Tsukada M, Physical. Review. B84, (2011) 195461