

## Yoshiyuki KAWAZOE

**Affiliation:** New Industry Creation Hatchery Center,  
Tohoku University

**Address:** 6-6-4 Aramaki aza Aoba, Aobaku, Sendai, 980-8579, Japan

**Phone:** +81-22-795-3121, **Fax:** +81-22-79503670

**E-mail:** kawazoe@e-workshop.co.jp



### Education

- 1972 – 1975 Dr. S. Tohoku University (Department of Physics)  
1970 – 1972 M.S. Tohoku University (Department of Chemistry)  
1966 – 1970 B.S. Tohoku University (Department of Chemistry)

### Professional Career

- 2015 – Present: Professor, New Industry Creation Hatchery Center, Tohoku University  
2012 – 2015: Professor Emeritus, New Industry Creation Hatchery Center, Tohoku University  
1990 – 2012: Professor, Institute for Materials Research, Tohoku University  
(1991 Visiting Professor at University of California at Berkeley)  
(2004-2007 Director, Computer Center, Tohoku Univ.)  
1981 – 1990: Associate Professor, Education Center for Information Processing, Tohoku University  
(1986: Invited Professor at WACAE, Australia)  
1975 – 1981: Research Associate, College of Arts and Sciences, Tohoku University  
(1981: Invited researcher at Max Planck Institute, Germany)

### Selected Publications

1. “Phase Diagrams and Physical Properties of Nonequilibrium Alloys”  
**Chief Editor**, Springer-Verlag (1997~).
2. “Materials Design by Computer Simulation”, **Y. Kawazoe**, K. Esfarjani, and K. Ohno, Springer(1999).
3. “Clusters and Nanoparticles”, **Y. Kawazoe**, T. Kondow, and K. Ohno, Springer-Verlag (2002).
4. “The Mechanisms for Pressure-Induced Amorphization of Ice I<sub>h</sub>”, J.S. Tse, D.D. Klug, C.A. Tulk, I. Swainson, E C. Svensson, C.-K. Loong, V. P. Shpakov, V.R. Belosludov, R.V. Belosludov and **Y. Kawazoe**, *Nature* 400, 647–649 (1999).
5. “Highly Controlled Acetylene Accommodation in a Metal-Organic Microporous Material”, R. Matsuda, R. Kitaura, S. Kitagawa, Y. Kubota, R.V. Belosludov, T.C. Kobayashi, H. Sakamoto, T. Chiba, M. Takata, **Y. Kawazoe** and Y. Mita, *Nature* 436, 238–241 (2005).
6. “Low-Temperature Phase Transformation from Graphite to *sp*<sup>3</sup> Orthorhombic Carbon”, J.-Tao Wang, C. Chen and **Y. Kawazoe**, *Phys. Rev. Lett.* **106**, 075501/1-4 (2011).
7. “Negatively curved cubic carbon crystals with octahedral symmetry”, M. Tagami, Y.-Y. Liang, H. Naito, **Y. Kawazoe**, and M. Kotani, *Carbon* 76, 266–274 (2014).
8. Penta-graphene: A new carbon allotrope”, S. H. Zhang, J. Zhou, Q. Wang, X. S. Chen, **Y. Kawazoe**, P. Jena, *PNAS* 112, 2372–2377 (2015).

More than 50 books and more than 1,000 ISI journal papers with more than 20,000 total citations with h-index of 61.

### Research Interests

1. Basics in theoretical materials science
2. Development of first principles calculation formulation and software
3. New nanocarbon allotropes
4. Gas storage materials (Hydrogen, CO<sub>2</sub>, etc. in Clathrate and MOF)