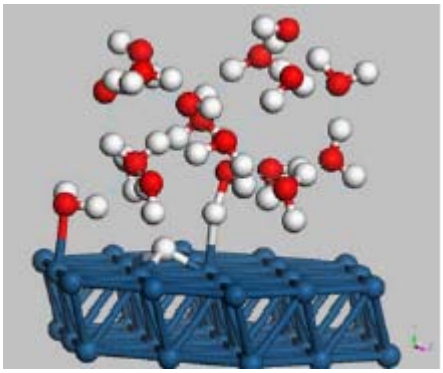
Yasuyuki Ishikawa

Quantum Simulator

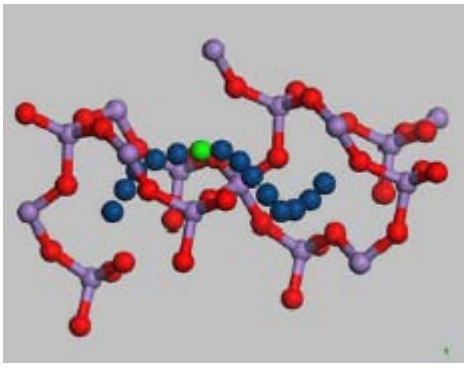
University of Puerto Rico, Río Piedras Campus

Biography

Ishikawa is an expert on theoretical simulation of the properties/reactivity of atoms, molecules, and nanoscale materials at various interfaces. After receiving a Ph.D. degree in Chemistry from the University of Iowa in 1976, he conducted extensive postdoctoral research on many-body theories in the United States, Germany and Canada before joining the College of Natural Sciences of the University of Puerto Rico, Rio Piedras Campus. He has provided extensive expertise to develop the first-principles theoretical framework to analyze the atomistic mechanism for heterolytic reactions at the fuel cell electrode/electrolyte interface–theoretical simulations of the surface reactions in electrochemical cells (supported by NASA and ARL), and for the Li+ mobility and structural stability of high energy density electrodes for novel lithium storage batteries (supported by the United States Department of Education). The goal of these theoretical/computational studies is to develop the first-principles theoretical framework for unraveling the atomistic mechanism, enabling the design of the next-generation nanoscale materials.



H_2 oxidation at Pt(111)/water interface.



Li ion mobility in $LiMn_2O_4$ cathode.

Teams

Cluster II: Functional Nanostructures at the Interface, Cluster III: Multifunctional Nanostructures

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Education

- Ph.D. in Chemistry, University of Iowa (1976)

Appointments

1999–present	Visiting Research Scientist, University of Tokyo, Hongo, Tokyo, Japan
1990–present	Professor of Chemistry and the Chemical Physics Program, University of Puerto Rico, Rio Piedras Campus, San Juan, PR, United States

Publications

1. C. R. Cabrera, Y. Ishikawa, and R. Kinch, "A Density-functional Theory Study of the Water-gas Shift Mechanism on Pt/Ceria (111)", J. of Physical Chemistry C, (2009)
2. J. Hoffmann, Y. Ishikawa, C. Krantz, J. A. Santana, E. Traebert, and A. Wolf, "Atomic lifetime measurements on forbidden transitions of Al-, Si-, P-, and S-like ions", Journal of Physics B, 42, 025002 (2009)
3. Y. Ishikawa, N. K. Karan, R. S. Katiyar, J. J. Saavedra-Arias, and R. Thomas, "First Principles Computations Studies: Structural and Electrochemical Behavior of Layered Cathode Materials", ECS Transaction, 16, 9 (2009)
4. Y. Ishikawa, E. Traebert, and M. J. Vilkas, "n=3-3 transitions of Ne-like ions in the iron group, especially Ca10+ and Ti12+,", Physica Scripta, 79, 025301 (2009)
5. S. Das, Y. Ishikawa, R. S. Katiyar, R. Katiyar, J. J. Saavedra-Aries, R. Singhal, M. S. Tomar, and M. J. Vilkas, "Spinel LiMn2-xNixO4 cathode materials for high energy density lithium ion rechargeable batteries", Journal of Renewable and Sustainable Energy, in press (2009)
6. Y. Ishikawa and M. J. Vilkas, "A relativistic R-matrix close-coupling method based on the effective many-body", Physical Review A, 77, 052701 (2008)
7. Y. Ishikawa, I. Konuma, N. Kurita, T. Natsume, and T. Tsukamoto, "Density-functional calculations of hydrated structures and electronic properties for G-C and", THEOCHEM, 862, 122 (2008)
8. Y. Ishikawa, I. Komura, and T. TsukaMoto, "Density-functional calculations of hydrated structures and electronic properties for G-C and A-T base pairs", JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 862, 122 (2008)
9. Y. Ishikawa, E. Traebert, and M. J. Vilkas, "Electric-dipole 5s-5p transitions in promethiumlike ions", Physical Review A, 77, 042510 (2008)
10. Y. Ishikawa, E. Trabert, and M. J. Vilkas, "Electric-dipole 5s-5p transitions in promethiumlike ions", PHYSICAL REVIEW A, 77, 042510 (2008)
11. K. Dedachi, Y. Ishikawa, N. Kurita, T. Nakatsu, T. Natsume, and T. Tuskamoto, "Hybrid QM/MM calculations on the structure and electronic properties of hydrated RNA", THEOCHEM, 854, 70 (2008)
12. K. DEDACHI, Y. Ishikawa, N. KURITA, T. NAKATSU, T. NATSUME, and T. TSUKAMOTO, "Hybrid QM/MM calculations on the structure and electronic

properties of hydrated RNA base pair", JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 854, 70 (2008)

13. Y. Ishikawa and M. J. Vilkas, "Relativistic many-body calculations of excited-state energies and transition wavelengths for", Physical Review A, 78, 042501 (2008)
14. Y. Ishikawa, E. Traebert, and M. J. Vilkas, "Relativistic many-body Møller-Plesset perturbation theory calculations of the energy levels", At. Data Nucl. Data Tables, 94, 650 (2008)
15. C. R. Cabrera, Y. Ishikawa, and T. Morante-Catacora, "Sequential electrodeposition of Mo at Pt and PtRu methanol oxidation catalyst particles on", Journal of Electroanalytical Chemistry, 621, 103 (2008)
16. C. R. Cabrera, Y. Ishikawa, and T. Y. MORANTE-CATACORA, "Sequential electrodeposition of Mo at Pt and PtRu methanol oxidation catalyst particles on HOPG surfaces", JOURNAL OF ELECTROANALYTICAL CHEMISTRY, 621, 103 (2008)
17. C. R. Cabrera, Y. Ishikawa, J. J. Mateo, and D. A. Tryk, "Underpotential deposition of hydrogen on Pt(111): A combined direct molecular", Molecular Simulation, 34, 1065 (2008)
18. C. R. Cabrera, Y. Ishikawa, J. J. Mateo, and D. A. Tryk , "Underpotential deposition of hydrogen on Pt(111): a combined direct molecular dynamics/density functional theory study", MOLECULAR SIMULATION, 34, 1065 (2008)
19. Y. Ishikawa, E. Traebert, and M. J. Vilkas, "A tale of two lines: Searching for the 5s-5p resonance lines in Pm-like ion spectra", Journal of Physics Conf. Series,
20. Y. Ishikawa and J. A. Santana, "Effective collision strengths for electron-impact excitation of transitions within the ground", International Journal of Quantum Chemistry,
21. Y. Ishikawa, N. Kurita, T. Tsukamoto, and H. Wakabayashi, "Hole-transfer mechanism in hydrated DNA duplexes: Direct ab initio molecular dynamics", ECS Transaction,
22. Y. Ishikawa, J. A. Santana, and E. Traebert, "Multireference Moller-Plesset perturbation theory results on levels and transition rates in", Physica Scripta,

Grants

1. O. Auciello, C. R. Cabrera, M. J. Guinel, Y. Ishikawa, J. Jellinek, M. Jose-Yacamán, G. Morell, R. G. Raptis, and G. Sandi. FUNDAMENTAL SCIENCE OF NANOSTRUCTURED ELECTROCATALYSTS/ DIAMOND SUPPORTS FOR FUEL CELL APPLICATIONS, United States Department of Energy, Hydrogen, 3 years, October 2009, Single PI, Pending, $3,900,000.
2. A. J. Hernández, Y. Ishikawa, B. Luna, G. Morell, and R. G. Raptis. A Combined Experimental and Theoretical Approach for the Development of Selective Nanoporous Gas Sorbents for the Effective Restoration of Breathing Air in Crewed Space Craft, National Aeronautics and Space Administration, EPSCoR, 3 years, October 2009, Multiple PIs, Pending, $1,350,000.
3. K. Belashchenko, B. Bockelman, Z. Chen, F. Choobineh, M. Gómez, Y. Ishikawa, H. Li, J. Lu, A. R. Mayol, H. Ortiz-Zuazaga, K. Riley, W. Srisa-an, D.

Swanson, E. Tsymbal, J. Velev, X. Zeng, N. A. Zimbovskaya, and S. Zuloski-Benson. Collaborative Research: Adaptive Cyberinfrastructure for Computational Nanoscience, National Science Foundation, OIA - RESEARCH INFRASTRUCTURE IMPROV, 3 years, August 2009, Multiple PIs, Pending, $2,627,400.

4. F. M. Aliev, C. R. Cabrera, L. F. Fonseca, K. H. Griebenow, A. J. Hernández, Y. Ishikawa, R. S. Katiyar, M. M. Martínez, A. R. Mayol, G. Morell, W. Otaño, R. G. Raptis, and B. R. Weiner. Center for Advanced Nanoscale Materials (CANM) NASA University Research, National Aeronautics and Space Administration, URC, 5 years, October 2008, Multiple PIs, Approved, $6,000,000.
5. O. Auciello, S. Bader, D. Bonnell, S. Desu, L. F. Fonseca, M. Gómez, S. Hong, Y. Ishikawa, R. S. Katiyar, V. Makarov, A. R. Mayol, G. Morell, W. Otaño, R. Palai, O. J. Perales, A. Petford-Long, R. Ramesh, A. Rastogi, R. Thomas, and M. S. Tomar. Development and Understanding of Multifunctional Nanostructures for Spintronics and Magnetoelectrics Applications, United States Department of Energy, EPSCoR, 3 years, September 2008, Multiple PIs, Approved, $2,245,000.
6. C. R. Cabrera, Y. Ishikawa, R. S. Katiyar, G. Morell, and R. G. Raptis. Space Exploration Enabling Power Systems: Partnership to Develop the Fundamental Science at UPR and Perform the Corresponding Proof-of-Concept at NASA GRC, National Aeronautics and Space Administration, EPSCoR, 3 years, October 2007, Multiple PIs, Approved, $1,350,000.
7. P. X. Feng, Y. Ishikawa, G. Morell, and B. R. Weiner. Large area, ambient pressure synthesis of nanocomposite carbon films, United States Department of Defense, AFSOR, 3 years, October 2006, Multiple PIs, Approved, $500,000.

Presentations

1. Y. Ishikawa, J. Mateo, and J. Santana (March 2009) "A first-principles simulation of the electrochemical interface: Electrooxidation of molecular hydrogen and UPD states of H at Pt-electrode/water interface" in International Conference on Simulation and Dynamics for Nanoscale and Biological Systems.
2. D. S. Belen-Cordero, Y. Ishikawa, and J. Mateo (October 2008) "A first-principles simulation of the electrochemical interface: Electrooxidation of molecular hydrogen and UPD states of hydrogen at Pt-electrode/water interface" in PRIM - Pacific Rim ECS Meeting.