

## List of Publications: Etsuko Fujita

1. Carbon Dioxide Reduction by Pincer Rhodium  $\eta^2$ -Dihydrogen Complexes: Hydrogen Binding Modes and Mechanistic Studies by Density Functional Theory Calculations. K.-W. Huang, J. H. Han, C. B. Musgrave, and E. Fujita, *Organometallics*, accepted.
2. Reaction of NH<sub>3</sub> with Titania: N-doping of the Oxide and TiN formation. H. Chen, A. Nambu, W. Wen, J. Graciani, Z. Zhong, J. C. Hanson, E. Fujita, and J. A. Rodríguez, *J. Phys. Chem. B*, accepted.
3. Direct Measurements of Rate Constants and Activation Volumes for the Binding of H<sub>2</sub>, D<sub>2</sub>, N<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and CH<sub>3</sub>CN to W(CO)<sub>3</sub>(PCy<sub>3</sub>)<sub>2</sub>: Theoretical and Experimental Studies with Time-Resolved Step-Scan FTIR and UV-vis Spectroscopy. D. C. Grills, R. van Eldik, J. T. Muckerman, and E. Fujita, *J. Am. Chem. Soc.*, **2006**, 128, 15728-15741.
4. N-doping of TiO<sub>2</sub>(110): Photoemission and Density Functional Studies, A. Nambu, J. Graciani, J.A. Rodriguez, Q. Wu, E. Fujita, and J. Fernandez-Sanz, *J. Chem. Phys.* **2006**, 125, 094706.
5. Kinetic Studies of the Photoinduced Formation of Transition Metal-Dinitrogen Complexes Using Time-Resolved Infrared and UV-vis Spectroscopy. D. C. Grills, K.-W. Huang, J. T. Muckerman, and E. Fujita, *Coord. Chem. Rev.* **2006**, 250, 1681-1695.
6. Transition State Characterization for the Reversible Binding of Dihydrogen to Bis(2,2'-bipyridine)rhodium(I) from Temperature- and Pressure-Dependent Experimental and Theoretical Studies. E. Fujita, B. S. Brunschwig, C. Creutz, J. T. Muckerman, N. Sutin, D. J. Szalda, R. van Eldik, *Inorg. Chem.* **2006**, 45, 1595 - 1603.
7. Carbon-to-Metal Hydrogen Atom Transfer: Direct Observation Using Time-Resolved Infrared Spectroscopy. J. Zhang, D. C. Grills, K.-W. Huang, E. Fujita, R. M. Bullock, *J. Am. Chem. Soc.* **2005**, 127, 15684-15685.
8. Reaction of Hydroxymethyl and Hydride Complexes in Water: Synthesis, Structure and Reactivity of a Hydroxymethyl-Cobalt Complex, C. Creutz, M. H. Chou, E. Fujita, and D. J. Szalda, *Coord. Chem. Rev.* **2005**, 249, 375-390
9. Why is Re-Re Bond Formation/Cleavage of [Re(bpy)(CO)<sub>3</sub>]<sub>2</sub> Different from that of [Re(CO)<sub>5</sub>]<sub>2</sub>? Experimental and Theoretical Studies on the Dimers and Fragments, E. Fujita and J.T. Muckerman, *Inorg. Chem.*, **2004**, 43, 7636-7647
10. Spectroscopic Characterization of Intermediates in CO<sub>2</sub> Reduction with Rhenium Photocatalysts, E. Fujita, Y. Hayashi, S. Kita and B. S. Brunschwig, In *Studies in Surface Science and Catalysis*, Vol. 153, pp 271-276, Elsevier, Amsterdam, 2004.

11. Characterization of Transit Species and Products in Photochemical Reactions of Re(dmb)(CO)<sub>3</sub>Et with and without CO<sub>2</sub>, K. Shinozaki, Y. Hayashi, B. S. Brunschwig, and E. Fujita, *Res. Chem. Intermed.*, in press.
12. Involvement of a Binuclear Species with the Re-C(O)O-Re Moiety in CO<sub>2</sub> Reduction Catalyzed by Tricarbonyl Rhenium(I) Complexes with Diimine Ligands: Strikingly Slow Formation of the Re-Re and Re-C(O)O-Re Species from Re(dmb)(CO)<sub>3</sub>S (dmb = 4,4'-dimethyl-2,2'-bipyridine, S = Solvent), Y. Hayashi, S. Kita, B. S. Brunschwig, and E. Fujita, *J. Am. Chem. Soc.* **2003**, *125*, 11976-11987.
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