

## DAFTAR PUSTAKA

- Anderson, A.B. 1981. Reactions and structures of water and oxygen covered Pt(111) and Fe(100). *Surf. Sci.* **105**. 159.
- Attard, G. A., Hazzazi, O., Wells, P. B., Climent, V., Herrero, E., Feliu, J. M., 2004, On the global and local values of the potential of zero total charge at well-defined platinum surfaces: stepped and adatom modified surfaces, *Journal of Electroanalytical Chemistry, Journal of Electroanalytical Chemistry* **568**, 329-342.
- Bernas, A., Ferradini, C., Jay-Gerin, J. P. 1997. On the Electronic Structure of Liquid Water: Facts and Reflections. *Chem. Phys.* **222**. 151.
- Blöch, P. E. 1994. Projector augmented-wave method. *Phys. Rev. B.* **50**. 17953
- Born M., dan Oppenheimer R. 1927. Zur Quantentheorie der Molekeln. *Ann. Phys.* **84**. 457.
- Born M., dan Oppenheimer R., 1927, "Zur Quantentheorie der Molekeln", *Ann. Phys.* **84**, 457.
- Cahyanto, W. T., Escano, M. C. S., Arevalo, R. L., dan Kasai, H., 2011, "Pt (111)-alloy surfaces for non-activated OOH dissociation", *e-J. Surf. Sci. Nanotech.* **9**, 325.
- Cahyanto, W.T., Widanarto, W., Effendi, M., Hamdi, M. R., 2015. *Interaction of methanol and its dehydrogenation species with Pt-alloy surfaces*. 2nd Padjajaran International Physics Symposium 2015 (PIPS-2015). 1-2 September 2015. Unpad: Bandung.
- Callister, W. D. Jr. 2007. *Material Science and Engineering An Inroduction Sevent Edition*. New York: John Wiley & Sons.
- Coe, J. V., Earhart, A. D., Cohen, M. H., Hoffman, G. J., Sarkas, H. W., dan Bowen, K. H. 1997. Using Cluster Studies to Approach the Electronic Structure of Bulk Water: Reassessing the Vacuum Level, Conduction Band Edge, and Band Gap of Water. *J. Chem. Phys.* **107**. 6023.
- Couto, P. C. D., Guedes, R. C., Cabral. B. J. C., dan Simões, J. A. M. 2003. The Hydration of the OH Radical: Microsolvation Modeling and Statistical Mechanics Simulation. *J. Chem. Phys.* **119**. 7344.
- Csaszar, A., Gábor, C., Tibor, T., Jonathan, T., Viktor, S., Sergei, V. S., Nikolai, F. Z., dan Oleg, L. P. 2005. On equilibrium structures of the water molecule. *J. Chem. Phys.* **122(21)**. 214305.

- Elba, C. G. 2017. "Studi Teoritik Adsorpsi H<sub>2</sub>O pada Permukaan PtRU(111) dengan Metode *Density Functional Theory*". *Skripsi*. Fakultas Matematika dan Ilmu Pengetahuan Alam UNSOED Purwokerto.
- Elina, Y. 2016. "Studi Teoritik Adsorpsi H<sub>2</sub>O pada Permukaan Pt(111) dengan Metode *Density Functional Theory*". *Skripsi*. Fakultas Matematika dan Ilmu Pengetahuan Alam UNSOED Purwokerto.
- Faraj, A. A. 2012. *DFT study of hydrogen adsorption and desorption at Pt edges and terraces for microfacets of varying sizes*. Tesis. Reykjavik: University Of Iceland.
- Gates, B. C., Katzer, J. R., dan Schuit G. C. A., 1979, "*Chemistry of catalytic processes*", McGraw-Hill Book Company, New York.
- Goulet, T., Bernas, A., Ferradini, C., dan Gerin, J. P. J. 1990. On the Electronic Structure of Liquid Water: Conduction-Band Tail Revealed by Photoionization Data. *Chem. Phys. Lett.* **170**. 5.
- Grand, D., Bernas, A., dan Amouyal, E. 1979. Photoionization of Aqueous Indole; Conduction Band Edge and Energy Gap in Liquid Water. *Chem. Phys.* **44**. 73.
- Hartanto, S., Sri, H., Lin, M., dan Latifah. 2007. Pengaruh Silika Pada Membran Elektrolit Berbasis Polietilena Eter Keton. *Jurnal Sains Materi Indonesia*. **8(3)**. 205-208.
- Ladelta V. 2007. *Direct Methanol Fuel Cell (DMFC): Baterai Laptop Tanpa Charger*, <http://www.chem-is-try.org>, diunduh tanggal 1 April 2016.
- Laasonen, K., Sprik, M., Parrinello, M., dan Car, R. 1993. Ab Initio Liquid Water. *J.Chem. Phys.* **99**. 11.
- Lee, J. G. 2012. *Computational Materials Science An Introduction*. New York: CRC Press.
- Mc. Cash. E. M. 2001. *Surface Chemistry*. Oxford : Oxford University Press.
- McCloskey, J. N. 2012. *A Density Functional Theory Study of the Surface Species on a Platinum-Ruthenium Catalyst used in a Methanol Fuel Cell*. Tesis. Worcester: Worcester Polytechnic Institute.
- Meng, S., Wang, E. G., dan Shiwu, G. 2004. Water adsorption on metal surfaces: A general picture from density functional theory studies. *Phy. Rev. B.* **69**. 195404.
- Monkhorst, H. J., dan Pack, J. D. 1976. On Special Points for Brillouin Zone Integrations. *Phys. Rev. B.* **13**. 5188.

- Morante-Catacora, T. Y., Ishikawa, Y., dan Cabrera, C. R., 2008, "Sequential electrodeposition of Mo at Pt and PtRu methanol oxidation catalyst particles on HOPG surfaces", *J. Electroanal. Chem.* **621**, 103
- Othman, M. H. D., Ismail, A. F., dan Mustafa, A. 2010. Recent Development of Polymer Electrolyte Membranes for Direct Methanol Fuel Cell Application. *Malaysian Polymer Journal.* **5(2)**. 1-36.
- Parravicini, G. P., dan Resca, L. 1973. Electronic States and Optical Properties in Cubic Ice. *Phys. Rev.* **8**. 6.
- Perdew, J. P., Burke, K., dan Ernzerhof, M. 1996. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **77(18)**. 3865.
- Perdew, J. P., Chevary, J. A., Vosko, S. H., Jackson, K. A., Pederson, M. R., Singh, D. J., dan Fiolhais, C. 1992. Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation. *Phys. Rev. B.* **46**. 6671.
- Pickett, W. E., 1985. Pseudopotential methods in condensed matter applications. *Comm. Solid State Phys.* **12**. 57.
- Pirovano, M. V. Ganduglia, V. Natoli and M. H. Cohen, J. Kudrnovsky dan I. Turek. 1996. *Potential, core-level, and d band shift at transition-metal surface.* *Journal of Physics.* **54(12)**. II
- Siagian, T. H. 2017. "Kajian Teoritik Adsorpsi H<sub>2</sub>O pada Permukaan PtRu(111) dengan Metode *Density Functional Theory*". *Skripsi.* Fakultas Matematika dan Ilmu Pengetahuan Alam UNSOED Purwokerto.
- Sulitayani, E.T. 2012. *Teori Fungsional Densitas dan Penerapannya pada Struktur Atom.* Prosiding Pertemuan Ilmiah XXVI HFI Jateng & DIY. 14 April 2012. Purworejo.
- Vaghari, H., Malmiri, H. J., Berenjian, A., dan Anarjan, N. 2013. Recent Advances in Application of Chitosan in Fuel Cells. *Sustainable Chemical Processes.* **1**. 16.
- Yeh, K. Y. 2012. *Atomistic Modeling Of The Cathode/Electrolyte Interface In Proton Exchange Membrane Fuel Cells.* Disertasi. USA: The Pennsylvania State University.
- Zhao, J., Changhoon, J., dan Choong, K. R. 2006. Adlayers of Sb Irreversibly Adsorbed on Pt(111): An Electrochemical Scanning Tunneling Microscopy Study. *J. Phys. Chem.* **110**. 10814-10821.