

- Absor, M. A. U., 2015, *Density-functional theory based calculation of spin orbit interaction in ZnO*, PhD thesis, Kanazawa University, Ishikawa, Japan.
- Afifah, D. N., Marlina, L. A., Hutama, A. S., & Wijaya, K. (2022). *Theoretical studies on structure and dynamics of anatase TiO₂ (101)/H₂SO₄/H₂O interface in the early stage of titania sulfation*. *Structural Chemistry*, 33(4), 1341-1354.
- Alderman, O. L. G., Skinner, L. B., Benmore, C. J., Tamalonis, A., & Weber, J. K. R. (2014). *Structure of molten titanium dioxide*. *Physical Review B*, 90(9), 094204.
- Akharkhach, B., & Barhdadi, A. (2021, November). *First-principles DFT Investigation of the Photocatalytic Capability of Cl Doped Rutil TiO₂ as a Self-Cleaning Coating for Photovoltaic Panels*. In 2021 9th International Renewable and Sustainable Energy Conference (IRSEC) (pp. 1-6). IEEE.
- Ansari, J.R., Sunilbhai, C.A., dan Sadasivuni, K.K., 2022. *MXenes and their composites for energy storage and conversion*. *Mxenes and their Composites*, pp.201-240.
- Anshory, M., Hanna, M. Y., & Adhib Ulil Absor, M. (2020). *Layer dependence of electronic structure in SnSe using first principle study*. *Materials Today: Proceedings*, 44,3249–3252. <https://doi.org/10.1016/j.matpr.2020.11.507>
- Atambo, M. O., Varsano, D., Ferretti, A., Ataei, S. S., Caldas, M. J., Molinari, E., & Selloni, A. (2019). *Electronic and optical properties of doped TiO₂ by many-body perturbation theory*. *Physical Review Materials*, 3(4), 045401.
- Bagher, A. M., Vahid, M. M. A., & Mohsen, M. (2015). *Types of solar cells and application*. *American Journal of optics and Photonics*, 3(5), 94-113.
- Baizae, S. M., & Mousavi, N. (2009). *First-principles study of the electronic and optical properties of rutil TiO₂*. *Physica B: Condensed Matter*, 404(16), 2111–2116 <https://doi.org/10.1016/j.physb.2009.01.014>
- Balesa, B. A., Lawal, A., Dalhatu, S. A., Idris, B., & Bello, M. (2021). *First principles calculations of structural, electronic and optical properties of nitrogen-doped*

titanium dioxide for solar cells application. Communication in Physical Sciences, 7(4).

- Bayani, A., Gebhardt, J., & Elsässer, C. (2023). *Electronic bulk and surface properties of titanium dioxide studied by DFT-1/2*. Langmuir, 39(42), 14922-14934.
- Berardinelli, A., & Parisi, F. (2021). *TiO₂ in the food industry and cosmetics*. In *Titanium Dioxide (TiO₂) and Its Applications* (pp. 353-371). Elsevier.
- Chen, T., Hao, Y. N., Jin, F., Wei, M., Feng, J., Jia, R., ... & Ma, Y. (2018). *Origin of the deep band-gap state in TiO₂ (110): d d σ bonds between Ti-Ti pairs*. Physical Review B, 98(20), 205135.
- Ekuma, C. E., & Bagayoko, D. (2011). *Ab-initio electronic and structural properties of rutil titanium dioxide*. Japanese Journal of Applied Physics, 50(10 PART 1). <https://doi.org/10.1143/JJAP.50.101103>
- Esfandfard, S. M., Elahifard, M. R., Behjatmanesh-Ardakani, R., & Kargar, H. (2018). *DFT study on oxygen-vacancy stability in rutil/anatase TiO₂: Effect of cationic substitutions*. Physical Chemistry Research, 6(3), 547-563.
- Fang, M., Wang, Z., Gu, H., Song, B., Guo, Z., Zhu, J., Chen, X., Zhang, C., Jiang, H., & Liu, S. (2021). *Complex optical conductivity of Bi₂Se₃ thin film: Approaching two-dimensional limit*. Applied Physics Letters, 118(19). <https://doi.org/10.1063/5.0049170>
- Fujiwara, H., 2007. *Spectroscopic ellipsometry: principles and applications*. John Wiley & Sons.
- Gatou, M. A., Syrrakou, A., Lagopati, N., & Pavlatou, E. A. (2024). *Photocatalytic TiO₂-based nanostructures as a promising material for diverse environmental applications: a review*. Reactions, 5(1), 135-194.
- Geldasa, F. T., & Dejene, F. B. (2025). *Effects of S Doping and Oxygen Vacancy on the Physical Properties of Rutil TiO₂ for Photocatalysis Applications Based on Density Functional Theory Study*. Materials, 18(8). <https://doi.org/10.3390/ma18081688>
- Geldasa, F. T., Dejene, F. B., Kebede, M. A., Hone, F. G., & Jira, E. T. (2025). *Density*



functional theory study of Chlorine, Fluorine, Nitrogen, and Sulfur doped rutil TiO₂ for photocatalytic application. Scientific Reports, 15(1), 3390.
<https://doi.org/10.1038/s41598-024-84316-0>

Gong, S., & Liu, B. G. (2012). *Electronic structures and optical properties of TiO₂: Improved density-functional-theory investigation.* Chinese Physics B, 21(5).
<https://doi.org/10.1088/1674-1056/21/5/057104>

Hamdan, S., Wigglesworth, M. J., Muscetta, M., Ma, R., Helal, M. I., Martsinovich, N., Palmisano, G., & Vernuccio, S. (2025). *Unravelling the photoactivity of metal-loaded TiO₂ for hydrogen production: Insights from a combined experimental and computational analysis.* International Journal of Hydrogen Energy, 118, 394–406. <https://doi.org/10.1016/j.ijhydene.2025.03.184>

Han, X., & Shao, G. (2011). *Electronic properties of rutil TiO₂ with nonmetal dopants from first principles.* Journal of Physical Chemistry C, 115(16), 8274–8282.
<https://doi.org/10.1021/jp1106586>

Hartree, D.R., 1928, January. *The wave mechanics of an atom with a non-Coulomb central field. Part I. Theory and methods.* Mathematical Proceedings of the Cambridge Philosophical Society (Vol. 24, No. 1, pp. 89-110). Cambridge university press.

Hohenberg, P., dan Kohn, W., 1964. *Inhomogeneous electron gas.* Physical review, 136(3B), p.B864.

Hotta, S., 2020. *Mathematical Physical Chemistry: Practical and Intuitive Methodology.* Springer Nature.

Houska, J., Mraz, S., & Schneider, J. M. (2012). *Experimental and molecular dynamics study of the growth of crystalline TiO₂.* Journal of Applied Physics, 112(7). <https://doi.org/10.1063/1.4757010>

Janzeer, Y. (2013). *Surface modification of titanium and titanium alloys to enhance bone healing* (Doctoral dissertation, Guy's, King's and St. Thomas's School of Dentistry).

Jellison, G. E., Modine, F. A., & Boatner, L. A. (1997). *Measurement of the optical functions of uniaxial materials by two-modulator generalized ellipsometry: rutil*

Kang, X., Liu, S., Dai, Z., He, Y., Song, X., & Tan, Z. (2019). *Titanium dioxide: from engineering to applications*. Catalysts, 9(2), 191

Kang, M., Kim, S. W., & Park, H. Y. (2018). *Optical properties of TiO₂ thin films with crystal structure*. Journal of Physics and Chemistry of Solids, 123, 266–270. <https://doi.org/10.1016/j.jpics.2018.08.009>

Katsura, T., & Tange, Y. (2019). *A simple derivation of the Birch–Murnaghan equations of state (EOSs) and comparison with EOSs derived from other definitions of finite strain*. Minerals, 9(12). <https://doi.org/10.3390/min9120745>

Koči, L., Kim, D. Y., De Almeida, J. S., Mattesini, M., Isaev, E., & Ahuja, R. (2008). *Mechanical stability of TiO₂ polymorphs under pressure: Ab initio calculations*. Journal of Physics Condensed Matter, 20(34). <https://doi.org/10.1088/0953-8984/20/34/345218>

Kulish, V. V., & Huang, W. (2017). *Single-layer metal halides MX₂ (X = Cl, Br, I): Stability and tunable magnetism from first principles and Monte Carlo simulations*. Journal of Materials Chemistry C, 5(34), 8734–8741. <https://doi.org/10.1039/c7tc02664a>

Körner, W., & Elsässer, C. (2011). *Density functional theory study of dopants in polycrystalline TiO₂*. Physical Review B, 83(20), 205315.

Landmann, M., Rauls, E., & Schmidt, W. G. (2012). *The electronic structure and optical response of rutil, anatase and brookite TiO₂*. Journal of Physics Condensed Matter, 24(19). <https://doi.org/10.1088/0953-8984/24/19/195503>

Maier, S.A., 2007. *Plasmonics: fundamentals and applications*. New York: Springer.

Malashevich, A., Jain, M., & Louie, S. G. (2014). *First-principles DFT+ G W study of oxygen vacancies in rutil TiO₂*. Physical Review B, 89(7), 075205.

Marden, M.P., 2010. *Condensed Matter Physics*, USA, John Willey and Sons.

McDonnell, K. A., English, N. J., Rahman, M., & Dowling, D. P. (2012). *Influence of doping*

on the photoactive properties of magnetron-sputtered titania coatings: Experimental and theoretical study. Physical Review B, 86(11), 115306.4

- Millis, A.J., 2004. *Optical conductivity and correlated electron physics.* Strong interactions in low dimensions, pp.195-235.
- Mora-Fonz, D., Kaviani, M., & Shluger, A. L. (2020). *Disorder-induced electron and hole trapping in amorphous TiO₂.* Physical Review B, 102(5), 054205.
- Munef, R. A., Ghaleb, A. M., & Shihatha, A. T. (2021). *Study of Rutil TiO₂ band structures and optical properties using Density functional theory (DFT).* Tikrit Journal of Pure Science, 26(3), 75-83.
- Muscat, J., Swamy, V., & Harrison, N. M. (2002). *First-principles calculations of the phase stability of TiO₂.* Physical Review B - Condensed Matter and Materials Physics, 65(22), 2241121–22411215. <https://doi.org/10.1103/PhysRevB.65.224112>
- Nishat, S. S., Hossain, M. J., Mullick, F. E., Kabir, A., Chowdhury, S., Islam, S., & Hossain, M. (2021). *Performance analysis of perovskite solar cells using DFT-extracted parameters of metal-doped TiO₂ electron transport layer.* The Journal of Physical Chemistry C, 125(24), 13158-13166.
- Norvell, J. C., ALS-NIELSEN W Dietrich, J. O., Als-Nielsen, J., Rev, P., Als-, J., Dietrich, O.W., Essam, J. W., Fisher, M. E., Chem Phys, J., Hunter, D. L., Phys, J. C., Baker C Domb, G. A., & E Animalu, A. O. (1967). *Many-Electron Effects in the Optical Conductivity of Simple Metals* by Kubo Formula. In PHYSICAL REVIEW B (Vol. 153, Issue 2).
- Ozaki, T., et al. (2020). *User's Manual of OpenMX Ver. 3.9.* <http://www.OpenMX-square.org>
- Orhan, O. K., & O'Regan, D. D. (2020). *First-principles Hubbard U and Hund's J corrected approximate density functional theory predicts an accurate fundamental gap in rutil and anatase TiO₂.* Physical Review B, 101(24), 245137.
- Palfey, W. R., Rossman, G. R., & Goddard III, W. A. (2021). *Structure, Energetics, and Spectra for the Oxygen Vacancy in Rutil: Prominence of the Ti–HO–Ti Bond.* The Journal of Physical Chemistry Letters, 12(41), 10175-10181

Park, J.M., 2004, *Optical and Magneto-optic Kerr effects of MnBi, Ni₂MnGa*, PhD thesis, Iowa State University, Iowa, USA.

Perdew, J.P., Harbola, M.K., dan Sahni, V., 1988. *Generalized Gradient Approximations for Exchange and Correlation: Numerical Tests and Prospects*. Condensed Matter Theories: Volume 3, pp.235-247.

Qiu, B., Zhao, X., Hu, G., Yue, W., Ren, J., dan Yuan, X., 2018. *Optical properties of graphene/MoS₂ heterostructure: first principles calculations*. Nanomaterials, 8(11), p.962.

Qu, Z. W., & Kroes, G. J. (2006). *Theoretical study of the electronic structure and stability of titanium dioxide clusters (TiO₂)_n with n= 1– 9*. The Journal of Physical Chemistry B, 110(18), 8998-9007.

Rofiatun, N. (2013). *Preparasi dan karakterisasi titanium dioksida dalam lingkungan basa kuat natrium hidroksida*. Skripsi. Yogyakarta: Fakultas MIPA, Universitas Negeri Yogyakarta.

Sholl, D.S. dan Steckel, J.A., 2022. *Density functional theory: a practical introduction*. John Wiley & Sons.

Singh, B. P., Goyal, S. K., & Kumar, P. (2021). *Solar pv cell materials and technologies: Analyzing the recent developments*. Materials Today: Proceedings, 43, 2843–2849. <https://doi.org/10.1016/j.matpr.2021.01.003>

Sivasankar, S. M., Amorim, C. de O., & Cunha, A. F. da. (2025). *Progress in Thin-Film Photovoltaics: A Review of Key Strategies to Enhance the Efficiency of CIGS, CdTe, and CZTSSe Solar Cells*. In Journal of Composites Science (Vol. 9, Issue 3). Multidisciplinary Digital Publishing Institute (MDPI). <https://doi.org/10.3390/jcs9030143>

Smith, S. J., Stevens, R., Liu, S., Li, G., Navrotsky, A., Boerio-Goates, J., & Woodfield, B. F. (2009). *Heat capacities and thermodynamic functions of TiO₂ anatase and rutil: Analysis of phase stability*. American Mineralogist, 94(2–3), 236–243. <https://doi.org/10.2138/am.2009.3050>

- Soussi, A., Ait Hssi, A., Boujnah, M., Boulkadat, L., Abouabassi, K., Asbayou, A., Elfanaoui, A., Markazi, R., Ihlal, A., & Bouabid, K. (2021). *Electronic and Optical Properties of TiO₂ Thin Films: Combined Experimental and Theoretical Study*. Journal of Electronic Materials, 50(8), 4497–4510. <https://doi.org/10.1007/s11664-021-08976-8>
- Sta, I., Jlassi, M., Hajji, M., Boujmil, M. F., Jerbi, R., Kandyla, M., Kompitsas, M., & Ezzaouia, H. (2014). *Structural and optical properties of TiO₂ thin films prepared by spincoating*. Journal of Sol-Gel Science and Technology, 72(2), 421–427. <https://doi.org/10.1007/s10971-014-3452-z>
- Tang, H., Prasad, K., Sanjinès, R., Schmid, P. E., & Lévy, F. (1994). *Electrical and optical properties of TiO₂ anatase thin films*. Journal of Applied Physics, 75(4), 2042–2047. <https://doi.org/10.1063/1.356306>
- Thébaud, S., Adessi, C., & Bouzerar, G. (2019). *Investigating the high-temperature thermoelectric properties of n-type rutile TiO₂*. Physical Review B, 100(19), 195202.
- Troullier, N. dan Martins, J.L., 1991. *Efficient pseudopotentials for plane-wave calculations*. Physical review B, 43(3), p.1993.
- Tsetseris, L. (2011). *Configurations, electronic properties, and diffusion of carbon and nitrogen dopants in rutile TiO₂: A density functional theory study*. Physical Review B, 84(16), 165201.
- Vásquez, G. C., Karazhanov, S. Z., Maestre, D., Cremades, A., Piqueras, J., & Foss, S. E. (2016). *Oxygen vacancy related distortions in rutile TiO₂ nanoparticles: A combined experimental and theoretical study*. Physical Review B, 94(23), 235209.
- Wunderlich, W., Miao, L., Tanemura, M., Tanemura, S., Jin, P., Kaneko, K., Terai, A., Nabatova-Gabin, N., & Belkada, R. (2004). *Ab-initio calculations of the Optical band-gap of TiO₂ thin films*.
- Yu, X., Li, C., Ling, Y., Tang, T. A., Wu, Q., & Kong, J. (2010). *First principles calculations of electronic and optical properties of Mo-doped rutile TiO₂*. Journal of Alloys and Compounds, 507(1), 33–37. <https://doi.org/10.1016/j.jallcom.2010.07.195>



UNIVERSITAS
GADJAH MADA

Kajian Komputasional Struktur Elektronik dan Optik pada Sistem TiO₂ (001) Surface dengan Pendekatan

Density Functional Theory (DFT)

David Bandhaso, Moh. Adhib Ulil Absor, S.Si., M.Sc., Ph.D.; Prof. Solihun, S.Si., M.Sc., Ph.D.Sc.

Universitas Gadjah Mada, 2025 | Diunduh dari <http://etd.repository.ugm.ac.id/>

Zhao, L., Magyari-Köpe, B., & Nishi, Y. (2017). *Polaronic interactions between oxygen*

vacancies in rutile TiO₂. Physical Review B, 95(5), 054104