

DAFTAR PUSTAKA

- Ashcroft, N. W., & Mermin, N. D. (1976). *Solid State Physics*
- Brieman, L., Friedman, J. H., Olshen, R. A., & Stone, C. J. (1984). Classification and regression trees. wadsworth. *Inc. Monterey, California, USA*.
- Breiman, L. (2001). Random Forests. *Machine learning*, 45(1), 5-32.
- Butler, S. Z., Hollen, S. M., Cao, L., Cui, Y., Gupta, J. A., Gutiérrez, H. R., ... & Goldberger, J. E. (2013). Progress, challenges, and opportunities in two-dimensional materials beyond *graphene*. *ACS nano*, 7(4), 2898-2926.
- Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O., & Walsh, A. (2018). *Machine learning* for molecular and materials science. *Nature*, 559(7715), 547-555.
- Castro Neto, A. H., Guinea, F., Peres, N. M., Novoselov, K. S., & Geim, A. K. (2009). The electronic properties of *graphene*. *Reviews of modern physics*, 81(1), 109-162.
- Chen, T. (2016). XGBoost: A Scalable Tree Boosting System. *Cornell University*.
- Chhowalla, M., Shin, H. S., Eda, G., Li, L., Loh, K. P., & Zhang, H. (2013). The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets. *Nature Publishing Group*, 5(4), 263–275.
<https://doi.org/10.1038/nchem.1589>
- Chhowalla, M., Jena, D., & Zhang, H. (2016). Two-dimensional semiconductors for transistors. *Nature Reviews Materials*, 1(11), 1-15.
- Choudhary, M. K., V, A. R., S, G. S., & Ravindran, P. (2025). Composition and structure based GGA bandgap prediction using *machine learning* approach. *Advanced Theory and Simulations*, 8(12), e00771.
- Cohen, A. J., Mori-Sánchez, P., & Yang, W. (2008). Insights into current limitations of density functional theory. *Science*, 321(5890), 792-794.
- Doshi-Velez, F., & Kim, B. (2017). Towards a rigorous science of interpretable *machine learning*. *arXiv preprint arXiv:1702.08608*.
- Feng, S., & Wang, J. (2024). Prediction of Organic–Inorganic Hybrid Perovskite *Band gap* by Multiple *Machine learning* Algorithms. *Molecules*, 29(2), 499.
- Friedman, J. H. (2001). Greedy function approximation: a gradient boosting

machine. *Annals of statistics*, 1189-1232.

Gjerding, M. N., Taghizadeh, A., Rasmussen, A., Ali, S., Bertoldo, F., Deilmann, T., ... & Thygesen, K. S. (2021). Recent progress of the computational 2D materials database (C2DB). *2D Materials*, 8(4), 044002.

Haastrup, S., Strange, M., Pandey, M., Deilmann, T., Schmidt, P. S., Hinsche, N. F., ... & Thygesen, K. S. (2018). The Computational 2D Materials Database: *high-throughput* modeling and discovery of atomically thin crystals. *2D Materials*, 5(4), 042002.

Hastie, T., Tibshirani, R., & Friedman, J. (2009). The elements of statistical learning.

Himanen, L., Geurts, A., Foster, A. S., & Rinke, P. (2019). Data-driven materials science: status, challenges, and perspectives. *Advanced Science*, 6(21), 1900808.

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

Huo, S., Zhang, S., Wu, Q., & Zhang, X. (2024). Feature-assisted *machine learning* for predicting *band gaps* of binary semiconductors. *Nanomaterials*, 14(5), 445.

Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., ... & Persson, K. A. (2013). Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. *APL materials*, 1(1).

James, G. (2013). An introduction to statistical learning with applications in R.

Kittel, C. (2005). *Introduction to Solid State Physics* (8th ed.). Wiley.

Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Physical review*, 140(4A), A1133.

Linardatos, P., Papastefanopoulos, V., & Kotsiantis, S. (2020). Explainable ai: A review of *machine learning* interpretability methods. *Entropy*, 23(1), 18.

Lipton, Z. C. (2018). The mythos of model interpretability: In *machine learning*, the concept of interpretability is both important and slippery. *Queue*, 16(3), 31-57.

Lu, B., Xia, Y., Ren, Y., Xie, M., Zhou, L., Vinai, G., ... & Wong, P. K. J. (2024).

When *machine learning* meets 2D materials: a review. *Advanced Science*, 11(13), 2305277.

Lundberg, S. M., Erion, G., Chen, H., DeGrave, A., Prutkin, J. M., Nair, B., ... & Lee, S. I. (2020). From local explanations to global understanding with explainable AI for trees. *Nature machine intelligence*, 2(1), 56-67.

Ma, B., Martín, C., Kurapati, R., Bianco, A., Ma, B., Martín, C., Kurapati, R., & Degradation-by-design, A. B. (2020). *Degradation-by-design : how chemical functionalization enhances the biodegradability and safety of 2D materials*
To cite this version : HAL Id : hal-03001592 enhances the biodegradability and safety of 2D materials.

Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical review letters*, 77(18), 3865.

Pham, P. V., Do, H. B., Vasundhara, M., Nguyen, V. H., Nguyen, T., Van Bui, H., ... & Park, J. H. (2024). Layer-by-layer thinning of two-dimensional materials. *Chemical Society Reviews*, 53(10), 5190-5226.

Ramasubramaniam, A. (2012). Large excitonic effects in monolayers of molybdenum and tungsten dichalcogenides. *Physical Review B—Condensed Matter and Materials Physics*, 86(11), 115409.

Ribeiro, I. C., Picoli, F. D., Moraes, P. I. R., Fonseca, A. F., Oliveira, L. N., Nogueira, A. F., & Da Silva, J. L. (2025). Impact of Thin Film Thickness on the Structural, Energetic and Optoelectronic Properties of Two-Dimensional FPEA2 (MA_{n-1}) Pb_n I3_{n+1} Perovskites. *ACS Applied Energy Materials*, 8(6), 3346-3359.

Rudin, C. (2019). Stop explaining black box *machine learning* models for high stakes decisions and use interpretable models instead. *Nature machine intelligence*, 1(5), 206-215.

Sabagh Moeini, A., Shariatmadar Tehrani, F., & Naeimi-Sadigh, A. (2024). *Machine learning-enhanced band gaps* prediction for low-symmetry double and layered perovskites. *Scientific Reports*, 14(1), 26736.

Schmidt, J., Marques, M. R., Botti, S., & Marques, M. A. (2019). Recent advances and applications of *machine learning* in solid-state materials

science. *npj computational materials*, 5(1), 83.

Sham, L. J., & Schlüter, M. (1983). Density-functional theory of the energy gap. *Physical review letters*, 51(20), 1888.

Shapley, L. S. (1953). A value for n-person games.

Wang, J., Wang, Y., Liu, X., & Wang, X. (2025). Prediction and Screening of Lead-Free Double Perovskite Photovoltaic Materials Based on *Machine learning*. *Molecules*, 30(11), 2378.

Ward, L., Agrawal, A., Choudhary, A., & Wolverton, C. (2016). A general-purpose *machine learning* framework for predicting properties of inorganic materials. *npj Computational Materials*, 2(1), 1-7.

Willmott, C. J., & Matsuura, K. (2005). Advantages of the Mean Absolute Error (MAE) over the Root Mean Square Error (RMSE) in assessing average model performance. *Climate research*, 30(1), 79-82.

Yao, W., Jia, W., Shen, R., Wang, J., Zhang, L., & Wang, X. (2025). *Machine learning* prediction of bandgap and formation energy in two-dimensional metal oxides. *Physica B: Condensed Matter*, 417821.

Zhang, J., Li, Y., & Zhou, X. (2023). Machine-learning prediction of the computed *band gaps* of double perovskite materials. *arXiv preprint arXiv:2301.03372*.