



## DAFTAR PUSTAKA

- Adant, C., Dupuis, M., & Bredas, J. L. (1995). Ab initio study of the nonlinear optical properties of urea: Electron correlation and dispersion effects. *Int. J. Quantum Chem.*, 56(29), 497-507. <https://doi.org/10.1002/qua.560560853>
- Abdellah, I. M., Eletmany, M. R., & Shafei, A. E. (2023). Exploring the impact of electron acceptor tuning in D- $\pi$ -A'- $\pi$ -A photosensitizers on the photovoltaic performance of acridine-based DSSCs: A DFT/TDDFT perspective. *Mater. Today. Comm.*, 35, 106170. <https://doi.org/10.1016/j.mtcomm.2023.106170>
- Abusaif, M. S., Fathy, M., Abu-Saied, M. A., Elhenawy, A. A., Kashyout, A. B., Selim, M. R., & Ammar, Y. A. (2021). New carbazole-based organic dyes with different acceptors for dye-sensitized solar cells: Synthesis, characterization, dssc fabrications and density functional theory studies. *J. Mol. Struct.*, 1225, 129297. <https://doi.org/10.1016/j.molstruc.2020.129297>
- Afolabi, S. O., Semire, B., & Idowu, M. A. (2021). Electronic and optical properties' tuning of phenoxazine-based D-A2- $\pi$ -A1 organic dyes for dye-sensitized solar cells. DFT/TDDFT investigations. *Heliyon*, 7(4), 6827. <https://doi.org/10.1016/j.heliyon.2021.e06827>
- Britel, O., Fitri, A., Benjelloun, A. T., Benzakour, M., & Mcharfi, M. (2022). Effect of additional  $\pi$ -spacers on the photovoltaic properties of organic dyes for efficient dye-sensitized solar cells: a theoretical study. *Rsrch. Chem. Intermed.*, 48(12), 5243-5264. <https://doi.org/10.1007/s11164-022-04850-2>
- Britel, O., Fitri, A., Benjelloum, A. T., Benzakour, M., & Mcharfi, M. (2023). New carbazole-based dyes for efficient dye-sensitized solar cells: a DFT insight. *Struct. Chem.*, 5, 1827-1842. <https://doi.org/10.1007/s11224-023-02122-2>
- Britel, O., Fitri, A., Benjelloun, A. T., Benzakour, M., & Mcharfi, M. (2022). Theoretical design of new carbazole based organic dyes for DSSCs applications. A DFT/TD-DFT insight. *J. Photochem. Photobiol. A Chem.*, 429, 113902. <https://doi.org/10.1016/j.jphotochem.2022.113902>
- Britel, O., Fitri, A., Benjelloun, A. T., Silmi, A., Benzakour, M., & Mcharfi, M.



- (2022). Theoretical investigation of the influence of  $\pi$ -spacer on photovoltaic performances in carbazole-based dyes for dye-sensitized solar cells applications. *J. Photochem. Photobiol. A Chem.*, 428. <https://doi.org/10.1016/j.jphotochem.2022.113870>
- Britel, O., Fitri, A., Benjelloun, A. T., Benzakour, M., & Mcharfi, M. (2022). Theoretical investigation by DFT and TDDFT the extension of  $\pi$ -conjugation of novel carbazole-based donor materials for bulk heterojunction organic solar cell applications. *J. Mol. Model.*, 28, 351. <https://doi.org/10.1007/s00894-022-05347-w>
- Fernandez, A. d. J., & Watson, J. (2022). Mexico's renewable energy innovation system: Geothermal and solar photovoltaics case study. *Environ. Innov. Soc. Transit.*, 43, 200-219. <https://doi.org/10.1016/j.eist.2022.04.004>
- Gao, F., Yang, C. L., Wang, M. S., Ma, X. G., & Liu, W. W. (2019). Theoretical studies on the feasibility of the hybrid nanocomposites of graphene quantum dot and phenoxazine-based dyes as an efficient sensitizer for dye-sensitized solar cells. *Spectroch. Acta. A Mol. Biomol. Spectrosc.*, 206, 216-223. <https://doi.org/10.1016/j.saa.2018.08.012>
- Green, M. A., Dunlop, E. D., Ebinger, J. H., Yoshita, M., Kopidakis, N., & Hao, X. (2020). Solar cell efficiency tables (version 56). *Prog. Photovoltaics Res. Appl.*, 28(7), 629-638. <https://doi.org/10.1002/pip.3303>
- Han, L., Zu, X., Cui, Y., Wu, H., Ye, Q., & Gao, J. (2014). Novel D-A- $\pi$ -A carbazole dyes containing benzothiadiazole chromophores for dye-sensitized solar cells. *Org. Electron.*, 15(7), 1536-1544. <https://doi.org/10.1016/j.orgel.2014.04.016>
- Hao, X. L., Zhao, J. G., Gao, J. R. & Han, L. (2015). Synthesis and photoelectric properties of carbazole sensitizing dyes based on a benzoic acid acceptor. *Acta Phys. -Chim. Sin.*, 31, 1977-1984. <https://www.whxb.pku.edu.cn/EN/10.3866/PKU.WHXB201509075>
- Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. *Physc. Rev.*, 136(3B), B864. B864. <https://doi.org/10.1103/PhysRev.136.B864>
- Jachak, M., Khopkar, S., Patel, K., Patil, Y., & Shankarling, G. (2021). Synthesis



- of novel d- $\pi$ -A chromophores: Effect of structural manipulations on photophysical properties, viscosity and DFT study. *J. Mol. Struct.*, 1233, 130086. <https://doi.org/10.1016/j.molstruc.2021.130086>
- Karthick, S. N., Hemalatha, K. V., Balasingnam, S. K., Clinton, F. M., Akshaya, S., & Kim, H. (2019). Dye-sensitized solar cells: history, components, configuration, and working principle. *Interfaces. Eng. Func. Mater.*, 1. <https://doi.org/10.1002/9781119557401.ch1>
- Kumar, V., & Chetti, P. (2023). The impact of aromatic  $\pi$ -spacers and internal acceptors in triphenylamine dyes for DSSCs: A DFT approach. *J. Mol. Graph. Model.*, 123, 108512. <https://doi.org/10.1016/j.jmgm.2023.108512>
- Kohn, W., & Sham, L. J. (1965). Self-Consistent Equations Including Exchange and Correlation Effects. *Physc. Rev.*, 140, A1133. <https://doi.org/10.1103/PhysRev.140.A1133>
- Lameirinhas, R. A. M., Torres, J. P. N., & Cunha, J. P. M. (2022). A Photovoltaic Technology Review: History, Fundamentals and Applications. *A2 Sol. Ener. Photovol. Sytms*, 15(5), 1823. <https://doi.org/10.3390/en15051823>
- Li, Y., Liu, J., Liu, D., Li, X., & Xu, Y. (2019). D-A- $\pi$ -A based organic dyes for efficient DSSCs: A theoretical study on the role of  $\pi$ -spacer. *Comput. Mater. Sci.*, 161, 163-176. <https://doi.org/10.1016/j.commatsci.2019.01.033>
- Li, Y., Li, X., & Xu, Y. (2020). Theoretical screening of high-efficiency sensitizers with D- $\pi$ -A framework for DSSCs by altering promising donor group. *Sol. Energy*, 196, 146-156. <https://doi.org/10.1016/j.solener.2019.11.092>
- Mandal, S., & Kandregula, G. R. (2023). A computational finding on the effect of  $\pi$ -conjugated acceptors in thiophene-linked coumarin dyes for potential suitability in DSSC application. *J. Photochem. Photobiol. A Chem.*, 435, 114300. <https://doi.org/10.1016/j.jphotochem.2022.114300>
- Mandal, S., Kandregula, G., & Ramanujam, K. (2020). Replacing aromatic  $\pi$ -system with cycloalkyl in triphenylamine dyes to impact intramolecular charge transfer in dyes pertaining to dye-sensitized solar cells application. *J. Photochem. Photobiol. A Chem.*, 403, 112862. <https://doi.org/10.1016/j.jphotochem.2020.112862>



- Marlina, L. A., Haryadi, W., Daengngern, R., & Pranowo, H. D. (2022). Molecular design of benzo[c][1,2,5]thiadiazole or thieno[3,4-d]pyridazine-based auxiliary acceptors through different anchoring groups in D- $\pi$ -A-A framework: A DFT/TD-DFT study. *J. Mol. Graph. Model.*, 113, 108148. <https://doi.org/10.1016/j.jmgm.2022.108148>
- Marques, F. C., Cortes, A. D. S., & Mei, P. R. (2019). Solar cells fabricated in upgraded metallurgical silicon, obtained through vacuum degassing and czochralski growth. *Silicon*, 11, 77-83. <https://link.springer.com/article/10.1007/s12633-018-9860-x>
- Mo, Y., Lin, Z., Wu, W., & Zhang, Q. (1966). Bond-distorted orbitals and effects of hybridization and resonance on C-C bond lengths. *J. Phys. Chem.*, 100(28), 11569-11572. <https://doi.org/10.1021/jp953433a>
- O'Regan, B., & Gratzel, M. (1991). A low-cost, high-efficiency solar cell based on dye-sensitized colloidal TiO<sub>2</sub> films. *Nature*, 353, 737-740. <https://doi.org/10.1038/353737a0>
- Pakravesh, F., Izadyar, M., & Arkan, F. (2021). Effect of electron donor and acceptor on the photovoltaic properties of organic dyes for efficient dye-sensitized solar cells. *Phys. Rev. B - Condens. Matter Mater. Phys.*, 609(43), 412815. <https://doi.org/10.1016/j.physb.2021.412815>
- Sham, L. J., & Khon, W. (1966). One-Particle Properties of an Inhomogeneous Interacting Electron Gas. *Phys. Rev.*, 145, 561. <https://doi.org/10.1103/PhysRev.145.561>
- Sharma, K., Sharma, V., & Sharma, S. S. (2018). Dye-Sensitized Solar Cells: Fundamentals and Current Status. *Nano. Rsrch. Lett.*, 13, 381. <https://link.springer.com/article/10.1186/s11671-018-2760-6>
- Tripathi, S., Kumar, V., & Chetti, P. (2022). Impact of internal (donor/acceptor) moieties and  $\pi$ -spacer in triphenylamine-based dyes for DSSCs. *J. Photochem. Photobiol. A Chem.*, 426, 113738. <https://doi.org/10.1016/j.jphotochem.2021.113738>
- Tripathi, A., Ganjoo, A., & Chetti, P. (2020). Influence of internal acceptor and thiophene based  $\pi$ -spacer in D-A- $\pi$ -A system on photophysical and charge



- transport properties for efficient DSSCs: A DFT insight. *Sol. Energy.*, 209, 194-205. <https://doi.org/10.1016/j.solener.2020.08.084>
- Wang, T., Hao, X., Han, L., Li, Y., Ye, Q., & Cui, Y. (2021). DA- $\pi$ -A carbazole dyes bearing fluorenone acceptor for dye sensitized solar cells. *J. Mol. Struct.*, 1226, 129367. <https://doi.org/10.1016/j.molstruc.2020.129367>
- Wazzan, N. A. (2019). A DFT/TDDFT investigation on the efficiency of novel dyes with ortho-fluorophenyl units (A1) and incorporating benzotriazole/benzothiadiazole/phthalimide units (A2) as organic photosensitizers with D-A2- $\pi$ -A1 configuration for solar cell applications. *J. Comput. Electrn.*, 18, 375-395. <https://link.springer.com/article/10.1007/s10825-019-01308-4>
- Wei, H., Shen, J., Liu, Y., Huang, T., Zhang, Q., Zhao, J., & Zhao, X. (2018). Synthesis and properties of organic sensitizers bearing asymmetric double donor - $\pi$ - acceptor chains for dye-sensitized solar cells. *Dye. Pigment.*, 149, 789-795. <https://doi.org/10.1016/j.dyepig.2017.11.042>
- Xu, Z., Li, Y., Zhang, W., Yuan, S., Hao, L., Xu, T., & Lu, X. (2019). DFT/TD-DFT study of novel T shaped phenothiazine-based organic dyes for dye-sensitized solar cells applications. *Spectrochim. Acta. A Mol. Biomol. Spectrosc.*, 212, 272-280. <https://doi.org/10.1016/j.saa.2019.01.002>
- Yu, X. L., Deng, J. Y., Chen, J. F., & Yang, H. Q. (2019). Prediction of  $^{13}\text{C}$  NMR Chemical Shifts of Quinolone Derivatives Based on DFT Calculations. *J. Struct. Chem.*, 60, 772-779. <https://link.springer.com/article/10.1134/S0022476619050093>