International Journal of Academic Multidisciplinary Research (IJAMR)
ISSN: 2643-9670
Vol. 6 Issue 12, December - 2022, Pages: 295-300

Method of Band Gap Estimation with Aluminum Oxide under UV-VIS Electromagnetic Spectrum at Definite Adsorption Wavelengths.

Ahmed Sani.K[1], Olabimtan Olabode.H[2*] and Yahaya Yakubu[3].

[1]Department of Science Laboratory Technology,
Nigerian Building and Road Research Institute, North West Office Kano, Kano State, Nigeria.
[2] Department of Industrial and Environmental Pollution,
National Research Institute for Chemical Technology, Zaria Kaduna State, Nigeria.
[3]Department of Applied Chemistry, Kaduna Polytechnic, Kaduna State, Nigeria.

Corresponding author*: Olabode4angel@gmail.com

Abstract: *Alumina, commonly known as aluminum oxide, is frequently utilized in the manufacturing of superconducting materials due to its great thermal stability and simplicity of processing. Depending on the precise chemical make-up of the substance, the temperature at which an aluminum oxide superconductor turns superconductive can change. The focus of contemporary solid-state physics and chemistry is on creating materials with cutting-edge functionality. The pursuit of an ambient temperature superconductor (A-SC) is one of the oldest and most intriguing high-end goals, attracting research efforts from all over the world. Here, we describe the development of a modeling equation for the band gap values caused by UV-Vis electromagnetic radiation for aluminum oxide, an ideal room-temperature superconducting material, to be* $y = 0.0002x^2 - 0.124x + 22.73$ ($R^2=1$). *This method explains the discrepancies in the band gap values of 12.40, 6.20, and 4.13eV at 100, 200, and 300 nm as a function of wavelength and temperature in terms of UV spectrum irradiation. Eventually, the modeling equation highlights the theoretical foundation of the basic idea of low temperature (ambient) superconductor energy gaps for potential technical applications.*

Keywords: Energy gaps, superconductor, aluminum oxide, electromagnetic spectrum and photons.

1.0 INTRODUCTION

Heike Kammerlingh Onnes, a Dutch physicist, made the initial discovery of superconductors in 1911. Onnes was able to effectively liquefy helium by studying ultra-cold refrigerators [1]. On that particular day, he only succeeded in producing a few quantities of liquified helium, but this marked the beginning of his new investigation. He was able to use liquid helium to cool other materials down to absolute zero (0 Kelvin) [1]. In 1911, Onnes began looking into the electronic nature of metal at extremely low temperatures. It has long been understood that metal's resistance decreases when cooled below room temperature, but it was unclear what limiting value the resistance would reach if the temperature was dropped to a point extremely close to absolute zero due to the dissipation of the wire's resistance [2]. This suggested that electrical resistance would gradually decrease, making for better electrical conductors. The topic of superconductivity in physics has been interesting and difficult for about 75 years, with scholars working on its development for years. However, due to the low-temperature requirements of cryogenic superconductors, it has only recently gained popularity. Superconductivity is now being applied in many fields, including electronics, medicine, theoretical and experimental science, the military, transportation, and power generation [3]. Due to the discovery of high-temperature superconductors that can function at liquid nitrogen temperatures (77k), superconductivity is now well-recognized and accessible to most academics. As one of the frontiers of scientific research, any conductive materials that do not inhibit the conduction of electricity present unique and exciting opportunities for researchers to explore and experiment in this new and important field of physics. In addition to the fact that the limitations of superconductivity have not yet been reached, theories explaining its behavior appear to be constantly evolving [4.5]. Superconductors only begin to conduct electricity below a certain transition temperature, or Tc, which is typically just a few degrees above absolute zero. Electric current has been observed to flow for years without a potential difference in a ringed superconducting material with no discernible reduction. An "energy gap," also known as a "band gap," defines the energy range within a solid without an electronic state, such as insulators and semiconductors. The energy variance between the highest point around the valence boundary and that of the conduction segment is termed the band gap or energy gap. In superconductors, the band gap relates to the amount of power required to split a cooper pair of electrons and disrupt the superconducting state [6]. The band, or energy gap, is known to vary with temperature [7] and pressure [8] due to thermal expansion.

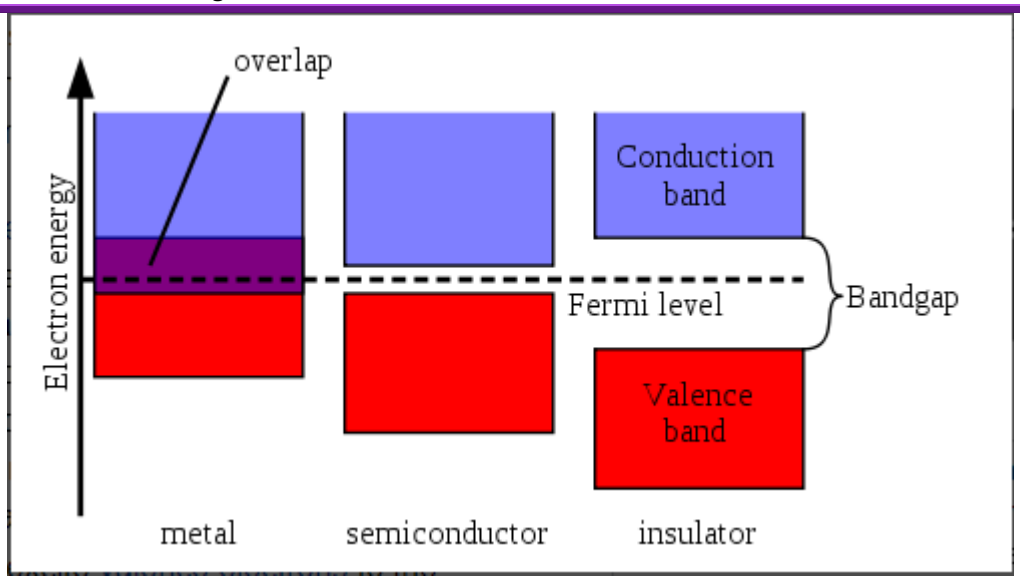

Figure 1. The valence and conduction bands of insulators, metals, and semiconductors. The Fermi level is the name given to the highest energy occupied electron orbital at absolute zero.

The trio of John Bardeen, Leon Cooper, and Robert Schrieffer effectively modeled the characteristics of type-1 superconductors in what is known as the BCS theory [9]. However, a core theoretical factor of their principle relates with the translation of electron pairs with fermi level to that of cooper pairs via collision against the crystal lattice. A tiny attraction between the electrons caused by lattice vibration is what leads to the pairing. This lattice's connection is known as a "phonon" [10]. The behavior of an interaction pair of electrons might differ significantly from that of a single electron, which is a fermion and is subject to the exclusion principle of Pauli [11]. More like a boson, which can condense to similar energy levels, the pair of electrons behave in this way as the electron pair's lower energy and energy gap above them, which is on the order of 0.001 eV, prevent the kind of collision contact that results in typical resistivity [12]. According to the behavior of superconductors, pairs of an electron are coupling through vast distances in nanometers, which is orders of magnitude greater than the cooper pair spacing in the lattice. These linked electrons are capable of condensation back to their ground state and acquiring the properties of a boson. Cooper pairs are formed when two electronic particles exchange phonons, which produces attractive interactions between them [13].

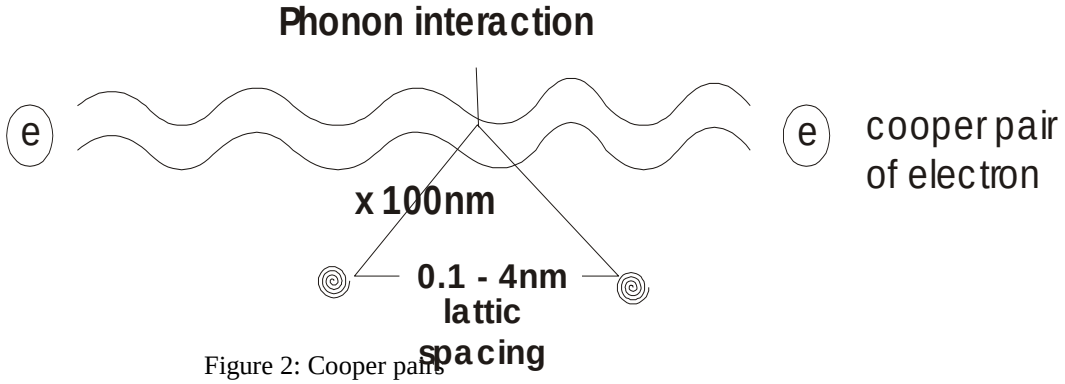

Figure 2: Cooper pairs

One option for mid-index coating materials is aluminum oxide (alumina, Al_2O_3), which is commonly used in the wavelength range between 7000 and 200 nm [4]. Additionally, because typical high-index oxide materials like titania, niobia, hafnia, tantala, and the like exhibit strong absorption in the Vacuum Ultraviolet/Deep Ultraviolet (VUV/DUV) spectral regions and are therefore unsuitable for interference coating design purposes, alumina emerges as an intriguing candidate for applications as a high index oxide VUV/DUV material [15]. This is especially important for applications involving lithography at 193 nm [16].

Due to its hardness, superior electrical insulation, useful optical properties, high surface area, and catalytic surface activity, aluminum oxide (Al_2O_3) is an industrial material of great interest, both for fundamental investigations and applications [17, 18]. Al_2O_3 single crystals, both pure and

doped, are well known for being superior materials for optics, optoelectronics, and laser applications [19]. With optical transmission across the UV to IR spectrums, pure Al_2O_3 is a tough material. Alumina films are applicable in multilayers with silicon dioxide (n = 1.48) for ultraviolet laser uses due to their low absorption below wavelengths of 300 nm [20]. Low-temperature substrates are suitable for the deposition of adherent coatings.

The optical absorption spectra are engaged in the determination of the optical transition, optical band gap, and band structure of crystalline and non-crystalline materials. The investigation of optically induced electronic transitions in many materials caused by the interaction of electromagnetic waves with valence electrons and raising them across the energy gap to the conduction band is commonly done by measuring the optical absorption coefficient close to the fundamental absorption edge [21]. Aluminum oxide is a wide-gap insulating material with a range of important technological applications, including in electronics, optics, and catalysis. The energy gap of a material is a measure of its ability to conduct electricity and is an important parameter in determining its electronic and optical properties. In this study, we present a modeled method for estimating the energy gap of Al_2O_3 under the ultraviolet-visible (UV-VIS) electromagnetic spectrum within 100-300 nm range at ambient temperature using a mathematical model to forecast its energy gap.

2.0 METHODOLOGY

The electrons are absorbing energy at a certain wavelength, as indicated by the UV/VIS spectroscopy absorption peak. When an electron absorbs energy, it transitions from its ground state to an excited state. The fact that electrons transit from their ground to their excited state indicates that a band gap exists in the material, which may be determined by the wavelength of absorption [22].

Energy Equation of Quantum Mechanics:

Energy (E) = Planks Constant (h) * Speed of Light (C) / Wavelength (λ)

Where, Energy (E) = Band gap,
Planks constant (h) = 6.626×10^{-34} Joules sec,
Velocity of Light (C) = 2.99×10^{-8} meter/sec and
Wavelength (λ) = Absorption peak value.
Where 1eV = 1.6×10^{-19} Joules (Conversion factor).

Using a UV-Vis spectrophotometer and predictively an aluminum powder with a purity of 99.99% and a defined particle size in standard solution, the absorption wavelengths of 100, 200, and 300 nm were the inputs for determining the UV spectroscopy band gap using the equation above. [23]

3.0 RESULTS AND DISCUSSION

Table 1. The UV spectroscopy energy gap profile of Aluminum oxide

Absorption wavelength (nm)	**Energy gap (eV)**	**Modeled equation** **y= energy gap** **x= absorption wavelength**	**Regression coefficient (R^2)**
100	12.40	$y = 0.0002x^2 - 0.124x + 22.73$	1
200	6.20		
300	4.13		

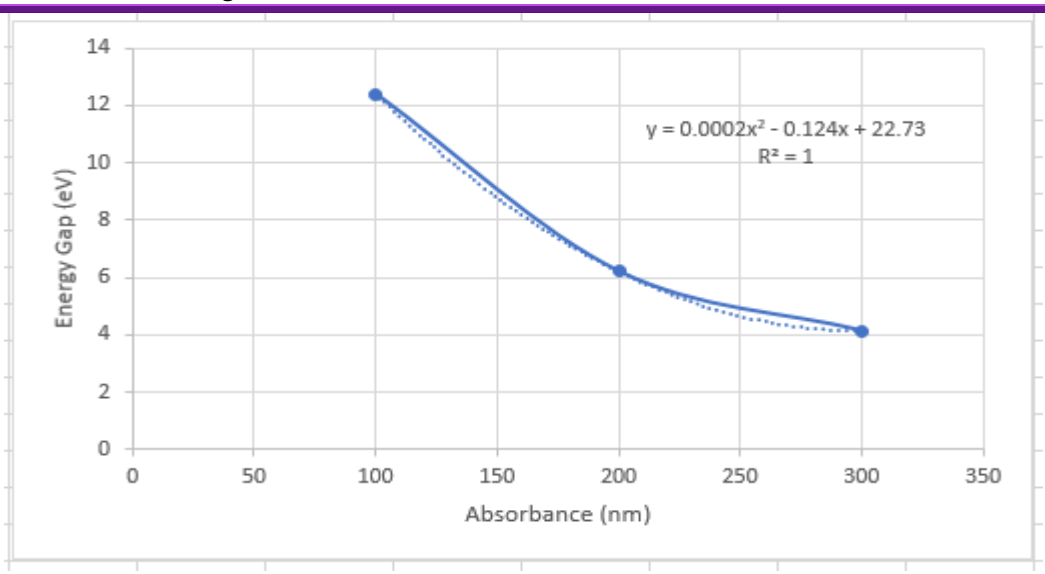

Figure 3. The plot of energy gap (Band Gap) of aluminum oxide at specified UV wavelength

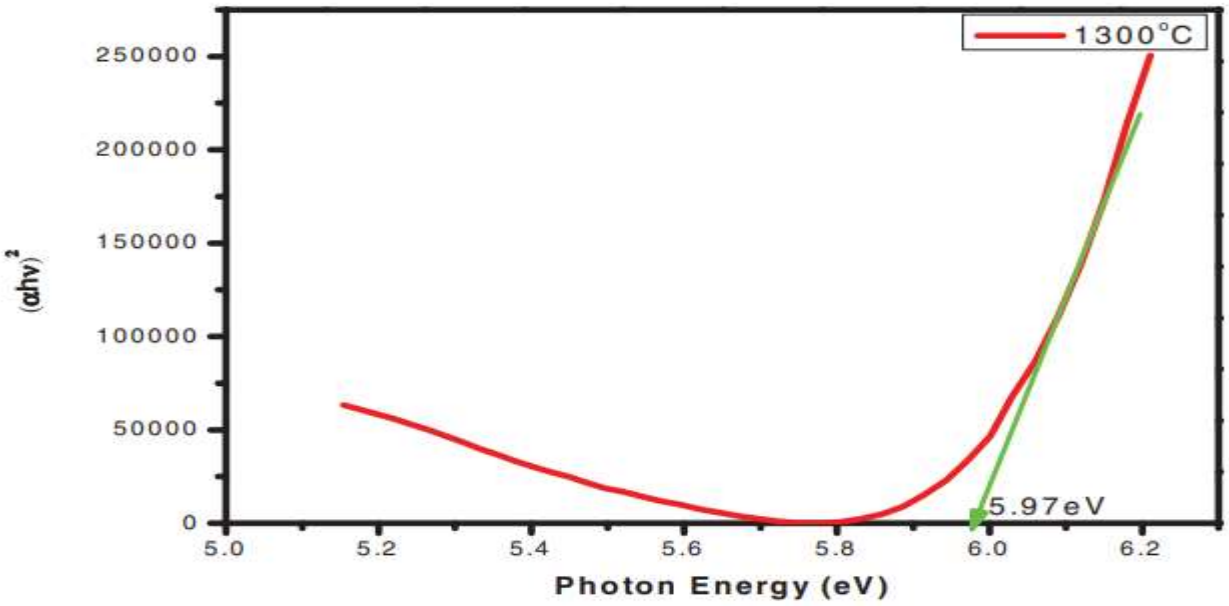

Figure 4. Band gap of Aluminum oxide

In general, the solution's concentration is directly correlated with how much light the material absorbs when the substance is present in the liquid. If the sample is solid, it must first be dissolved in a transparent solvent to be measured. The absorption peak in the UV-VIS spectrum suggests that the electrons are absorbing energy at a particular wavelength. The fact that electrons migrate from their ground to their excited state indicates that a band gap exists in the material, which may be determined by the wavelength of absorption.

Since the optical energy gap of the suitable sample's electronic structure was studied using the UV-VIS spectrum, the electronic changes inside the sample (aluminum oxide) caused absorption in the near UV range [24]. The UV-visible spectra of aluminum oxide nanoparticles displayed a band that was pushed towards the lower wavelength side, according to Nguyen *et al*. (2017) and Ghelani *et al*. (2022) [25],[26]. This tilt is related to the Al2O3 particles' regular organization, which was highly measurable in the synthesis. For alumina nanoparticles, Prashanth *et al*. (2015) discovered a comparable absorption band with an energy band of 5.25eV [27].

Thus, according to the quadratic model of ($y = 0.0002x^2 - 0.124x + 22.73$), the energy gap of Al_2O_3 technically spans between the wavelengths of 200 and 300 nm beneath the UV-Visible electromagnetic spectrum. A variety of complicated material properties may now be modeled from the ground up because of improvements in electronic structure approaches, software, and computational power. The study of

conventional superconductivity in particular has advanced significantly from generating hazy predictions about the critical temperature (Tc) to investigating pairing mechanisms and closing superconducting energy gaps.

Although it is still difficult to accurately anticipate superconducting qualities from scratch, most studies still rely on the semi-empirical McMillan or Allen-Dynes formulas to determine the critical temperature. The invention of the many-body Eliashberg theory, a generalization of the Bardeen-Cooper-Schrieffer microscopic theory of superconductivity, is largely responsible for the progress attained in the characterization of the superconducting state in materials with conventional pairing.

The frequency-dependent superconducting band gap is directly accessible using this cutting-edge theoretical approach, which is linked to Green's function formalism and provides a solution to a set of coupled diagrammatic equations for both electronic and phononic propagators. The method has been very helpful for resolving anisotropic Eliashberg equations, or equations that depend on band and crystal momentum. It has been utilized to examine the two-gap structure in MgB_2 and other fascinating superconductors since it can naturally resolve numerous gaps in the FS. Only with highly dense electron and phonon meshes to correctly sample the electron-phonon (e-ph) scattering processes close to the FS is the precise anisotropic description possible. To solve this computing problem, a first-principles interpolation method based on Wannier functions was developed. Utilizing the spatial allowance with an electronic-photon matrix system in the Wannier basis, the technique enables effective interpolation of those elements from a given uniform coarse grid to a desired arbitrarily dense Brillouin zone (BZ) grid at a significantly lower computational cost. It has also been suggested that a numerical method based on symmetric Helmholtz Fermi-surface harmonics (HFSH) is a reliable method for handling the anisotropy of the e-ph interaction in the Eliashberg equations.

The core concept is to substitute cheap sums over a few HFSH coefficients for BZ integrals in the k space. Even though these developments have made it possible to accurately represent the e-ph anisotropy from the ground up, the Coulomb correlation effects in the Eliashberg equations are still primarily handled by a single empirical parameter that only affects the region around the fermi's level. The pattern of the superconducting state in various classes of materials will be revealed by a description of the electron-electron (e-e) and electron-photon (e-ph) interactions on an equal footing.

In figure 4, where the absorption coefficient corresponding to the absorption edge (nm), hy is the photon energy, and is the constant proportionality, according to Bharthasaradhi and Nehru (2016), multiple reasons for this model are shown. The degree of the optical absorption margin is extrapolated using the plot of (ahy) 2 versus photon energy for direct permitted transition in the intercept at a D 0. The optical energy gap is thus calculated with the extrapolation of the linear component from Figure 6, which depicts the fluctuation of (ahn) 2 vs hn in the fundamental absorption region. Therefore, it is assumed that 5.67 eV represents the band gap [31].

4.0 CONCLUSION

Superconductors have a wide range of important applications in a variety of industries, including solar energy conversion (photoelectrochemical and photovoltaic solar cells, photocatalysis, and electrocatalysis), microelectronics (high-k, high-band-gap materials, resistive random access memory (ReRAM)), relative anticorrosive coatings, band or energy gap modeling of simple and complex oxides, and more. The prediction of band gap values of materials, even for the most advanced quantum mechanical approaches based on density functional theory, remains a difficult task despite the notable advances in computing a range of solid-state properties of various materials (DFT).

Therefore, to simulate the energy band for the manufactured alumina particles, the UV-irradiation approach is first and foremost regarded as an environmentally benign method with significant UV absorbance and perceived to be a reliable pathway.

Hence, we have presented a modeled method for estimating the energy gap of Al_2O_3 under the UV-VIS electromagnetic spectrum at definite adsorption wavelengths. Our results demonstrate the accuracy and reliability of this method, which can be used to characterize the electronic and optical properties of Al_2O_3 and other materials. Further studies are needed to investigate the effect of different parameters, such as temperature and pressure, on the energy gap of Al_2O_3 and other materials.

REFERENCES

1. Narlikar, A.V. (2014) “Onnes’ discovery and one hundred years of superconductors,” *Superconductors*, pp. 1–14. Available at: https://doi.org/10.1093/acprof:oso/9780199584116.003.0001.
2. “Electrical resistance of pure metal at very low temperatures. (1911). *Scientific American*, *72*(1863supp), 178-179. doi:10.1038/scientificamerican09161911-178bsupp
3. Applications of superconductivity. (2015). *Superconductivity*, 373-476. doi:10.1002/9783527686513.ch7
4. Sharma, R. G. (2021). A review of theories of superconductivity. *Superconductivity*, 123-160. doi:10.1007/978-3-030-75672-7_4
5. Hirsch, J. E., & Marsiglio, F. (2021). Nonstandard superconductivity or no superconductivity in hydrides under high pressure. *Physical Review B, 103*(13). doi:10.1103/physrevb.103.134505
6. Rahman, F., & Center, S. (2014). Solid-state lighting with wide band gap semiconductors. *MRS Energy & Sustainability, 1*(1). doi:10.1557/mre.2014.11
7. Omer, M. S., Karim, A. S., & Yousif, S. O. (2000). The temperature dependence of the energy gap of CDGEP2

Semiconductor. *Journal of Zankoy Sulaimani - Part A, 4*(1), 37-44. doi:10.17656/jzs.10063

8. Güler-Kılıç, S., & Kılıç, Ç. (2016). Pressure dependence of the band-gap energy in Bitei. *Physical Review B, 94*(16). doi:10.1103/physrevb.94.165203
9. Chávez, I., Grether, M., & De Llano, M. (2022). Superconductor superfluid density from the bardeen–cooper–schrieffer/bose crossover theory. *SN Applied Sciences, 4*(7). doi:10.1007/s42452-022-05074-0
10. Kłosowski, Ł, & Piwiński, M. (2020). Attraction between trapped ions and beams of electrons. *AIP Advances, 10*(1), 015028. doi:10.1063/1.5133999
11. Chakraborty, R., & Mazziotti, D. A. (2015). Structure of the one-electron reduced density matrix from the generalized Pauli Exclusion Principle. *International Journal of Quantum Chemistry, 115*(19), 1305-1310. doi:10.1002/qua.24934
12. MATAGA, N. (1994). Pioneering and developing exciplex chemistry. Part3. Energy gap dependences of electron transfer reactions and their roles as well as roles of solvent dependent exciplex structures which are of crucial importance for organic photochemical reaction mechanisms. *The Review of Laser Engineering, 22*(10), 809-816. doi:10.2184/lsj.22.809
13. Matsuo, M. (2013). Spatial structure of Cooper pairs in nuclei. *Fifty Years of Nuclear BCS*, 61-72. doi:10.1142/9789814412490_0005
14. Abyzov, A. M. (2019). Aluminum oxide and alumina ceramics (review). Part 1. Properties of al2o3 and commercial production of dispersed al2o3. *Refractories and Industrial Ceramics, 60*(1), 24-32. doi:10.1007/s11148-019-00304-2
15. IMAI, M., & NISHIKAWA, E. (2015). Comparison of etching effects using Deep ultraviolet (DUV) and vacuum ultraviolet/deep ultraviolet (VUV/duv) irradiation on multiwalled carbon nanotubes. *Journal of the Surface Finishing Society of Japan, 66*(10), 467-471. doi:10.4139/sfj.66.467
16. Philipsen, V., Jonckheere, R. M., Kohlpoth, S., & Torres, A. (2002). Defect printability for 100-nm design rule using 193-nm lithography. *SPIE Proceedings*. doi:10.1117/12.476978
17. Wei Qiang, L. (2014). Variation of structural and surface properties of RF sputtered aluminum oxide (al2o3) thin films due to the influence of annealing temperature and time. *International Journal of Materials Science and Applications, 3*(6), 404. doi:10.11648/j.ijmsa.20140306.29
18. Morajkar, P. P., & Fernandes, J. B. (2010). A new facile method to synthesize mesoporous γ-al2o3 of high surface area and catalytic activity. *Catalysis Communications, 11*(5), 414-418. doi:10.1016/j.catcom.2009.11.011
19. Kirm, M., Lushchik, A., Lushchik, C., Vielhauer, S., & Zimmerer, G. (2003). Luminescence of pure and doped al2o3 and mgo single crystals under inner-shell excitation. *Journal of Luminescence, 102-103*, 307-312. doi:10.1016/s0022-2313(02)00521-5
20. Yang, M., Gatto, A., & Kaiser, N. (2006). Optical thin films with high reflectance, low thickness and low stress for the spectral range from vacuum UV to near ir. *Journal of Optics A: Pure and Applied Optics, 8*(3), 327-332. doi:10.1088/1464-4258/8/3/016
21. Romanova, E., Parshina, N., Kochubey, V., Sukhanov, M., & Shiryaev, V. S. (2022). Optical properties of rear earth doped chalcogenide glasses near the fundamental absorption band edge. *2022 International Conference Laser Optics (ICLO)*. doi:10.1109/iclo54117.2022.9839921
22. Antonov, L. (2013). Absorption UV-vis spectroscopy and chemometrics: From qualitative conclusions to quantitative analysis. *Tautomerism*, 25-47. doi:10.1002/9783527658824.ch2
23. Singh, R., & Soni, R. K. (2014). Laser synthesis of aluminium nanoparticles in biocompatible polymer solutions. Applied Physics A, 116(2), 689–701. doi:10.1007/s00339-014-8487-z
24. Absorption of ultraviolet, visible, and near-infrared radiation. (2012). *Molecular Fluorescence*, 31-51. doi:10.1002/9783527650002.ch2
25. Nguyen, D., Lee, H., & Kim, I.-T. (2017). *Synthesis and Thermochromic Properties of Cr-Doped Al2O3 for a Reversible Thermochromic Sensor. Materials, 10(5), 476.* doi:10.3390/ma10050476
26. Ghelani, D., & Faisal, S. (2022). Synthesis and characterization of aluminium oxide nanoparticles. doi:10.22541/au.166490972.20428974/v1
27. Margine E R and Giustino F 2013 Anisotropic Migdal–Eliashberg theory using Wannier functions *Phys. Rev. B* **87** 024505
28. Giustino F, Cohen M L and Louie S G 2007 Electron–phonon interaction using Wannier functions *Phys. Rev. B* **76** 165108
29. Poncé S, Margine E R, Verdi C and Giustino F 2016 EPW: electron–phonon coupling, transport and superconducting properties using maximally localized Wannier functions *Comput. Phys. Commun.* **209** 116
30. Lafuente-Bartolome J, Gurtubay I G and Eiguren A 2020 Fully anisotropic superconductivity with few Helmholtz Fermi-surface harmonics *Phys. Rev. B* **102** 161107(R)
31. R. Bharthasaradhi & L.C. Nehru (2016) Structural and phase transition of α-Al2O3 powders obtained by co-precipitation method, Phase Transitions, 89:1, 77-83, DOI:10.1080/01411594.2015.1072628