Back in 2019, I published a research article in Physical Review B [1] that delved into the structural and electronic properties of bulk ZnS and small ZnS nanoclusters using a practical computational method called DFT+*U*. This method incorporates a Hubbard correction to enhance the accuracy of traditional DFT-GGA methods, particularly in determining material properties such as band gaps.

Our study revealed that the inclusion of the Hubbard correction term had a significant impact on the structural and electronic characteristics of bulk ZnS. We compared our findings with previous studies that employed GGA-based methods. Additionally, we utilized optimized Hubbard parameters to investigate the structural, electronic, and optical properties of ZnS nanoclusters of various sizes.

Our calculations involved analyzing properties like the density of states, band structures, bulk modulus, and effective masses for different crystal structures of bulk ZnS (zinc blende and wurtzite), and we compared these results with other research findings. Furthermore, we computed and compared the HOMO-LUMO gaps and cohesive energies of the ZnS nanoclusters using both DFT+*U* and traditional DFT methods. Remarkably, the results obtained from DFT+*U* were found to be in close agreement with those from Hybrid functionals like B3LYP. This success of the DFT+*U* method holds significant implications for high-throughput quantum mechanics, as it enables accurate predictions of material properties at a reduced computational cost.

In summary, our research emphasizes the importance of employing practical and effective computational methods such as DFT+*U* to achieve precise predictions of material properties. Furthermore, it highlights the necessity for further investigations aimed at enhancing traditional DFT techniques to facilitate more efficient and accurate predictions.

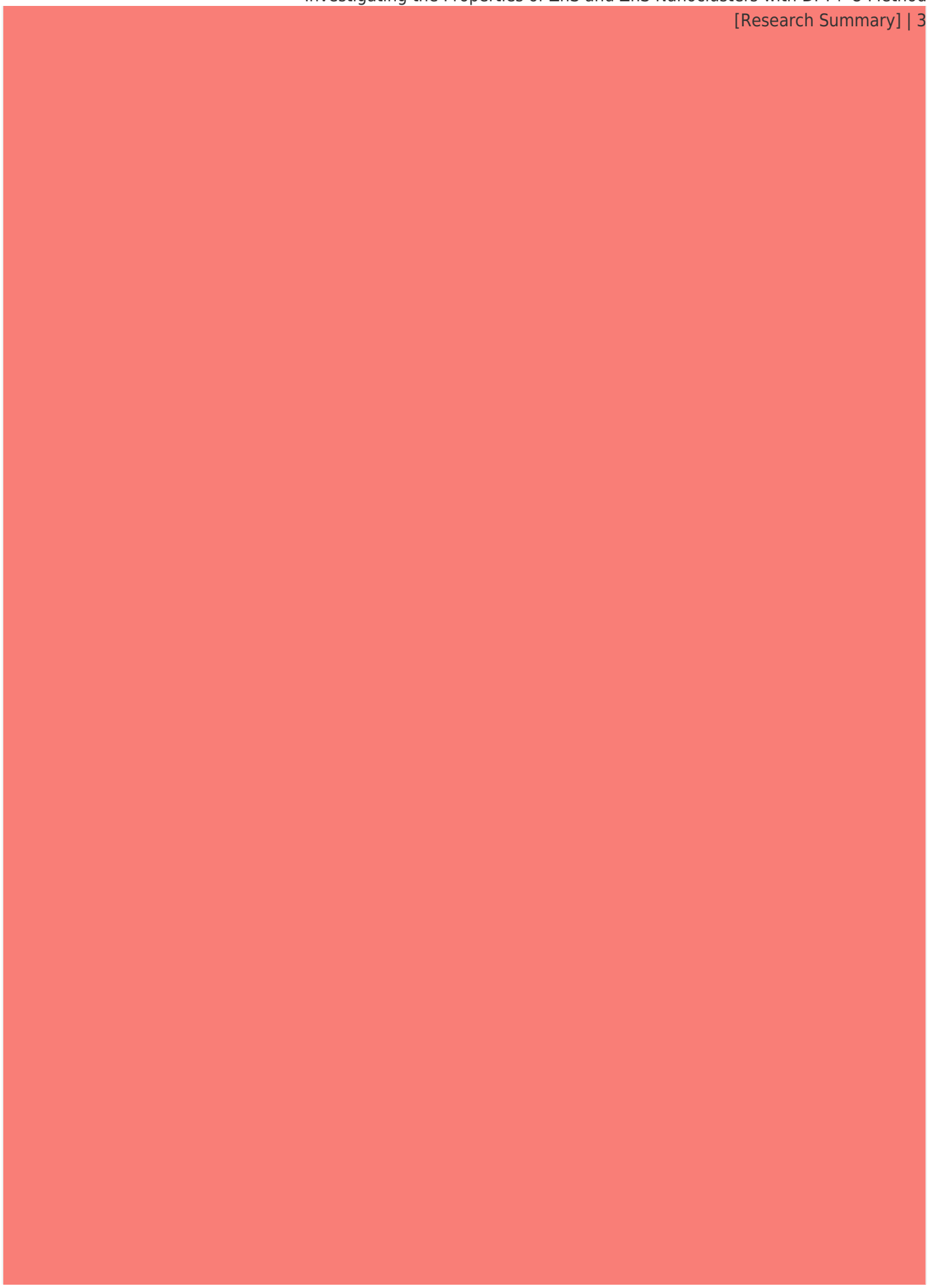
References

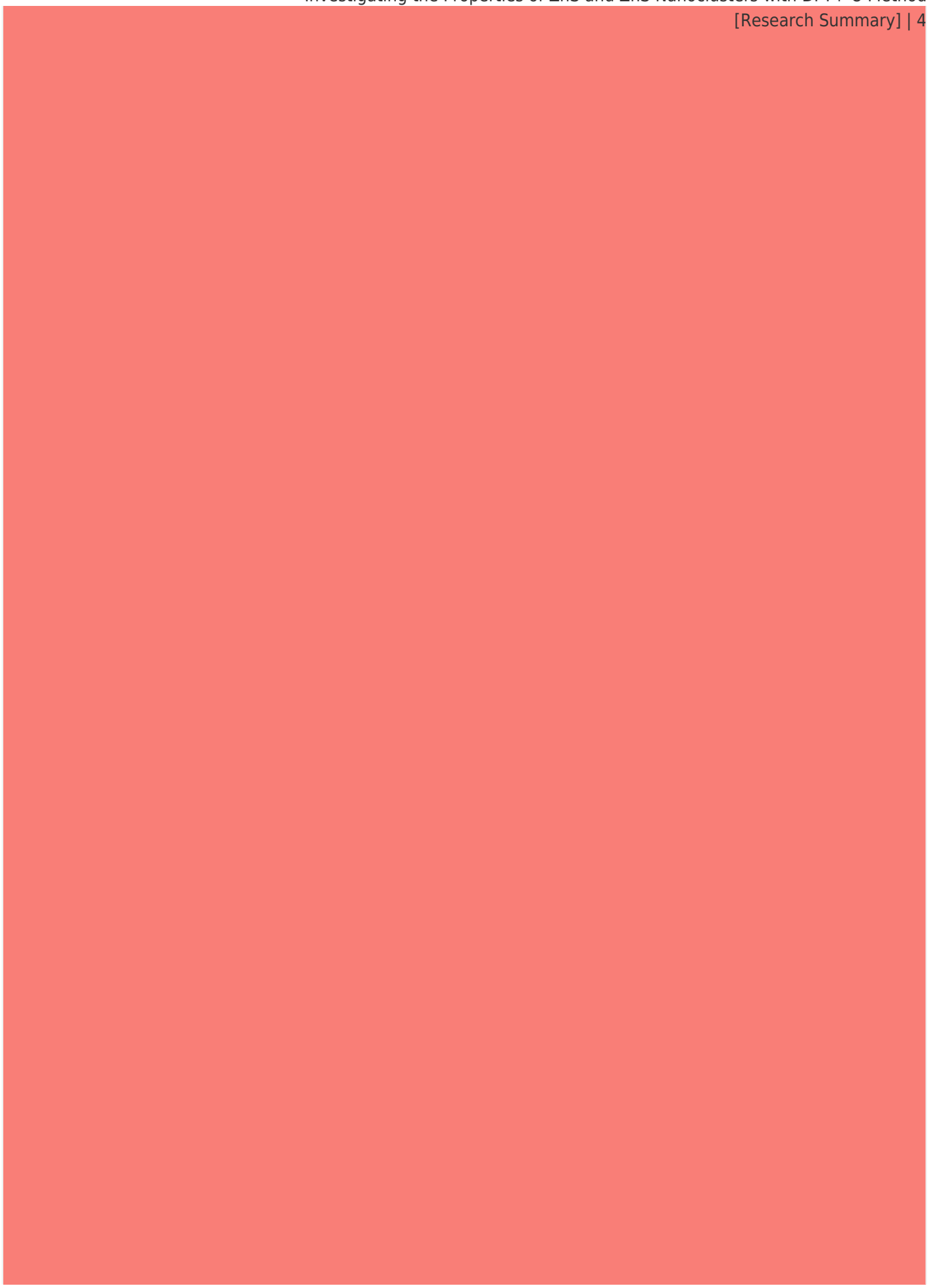
[1] M. Sharma, D. Mishra, and J. Kumar, *First-Principles Study of the Structural and Electronic Properties of Bulk ZnS and Small ZnnSn Nanoclusters in the Framework of the DFT+U method*, Physical Review 100, 045151 (2019).

Manas Sharma

I’m a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

manas.bragitoff.com/





Share this:

Click to share on Facebook (Opens in new window)

Click to share on Twitter (Opens in new window)

Click to share on WhatsApp (Opens in new window)

Click to share on Pinterest (Opens in new window)

Click to share on Reddit (Opens in new window)

Click to share on LinkedIn (Opens in new window)

Click to email a link to a friend (Opens in new window)

Click to print (Opens in new window)

Click to share on Tumblr (Opens in new window)

Click to share on Pocket (Opens in new window)

Click to share on Telegram (Opens in new window)

[wpedon id="7041" align="center"]