



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.

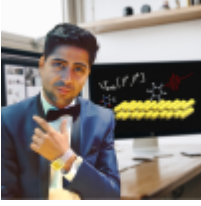
Our study revealed that the inclusion of the Hubbard correction term had a significant impact on the structural and electronic characteristics of bulk ZnS. We compared our findings with previous studies that employed GGA-based methods. Additionally, we utilized optimized Hubbard parameters to investigate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

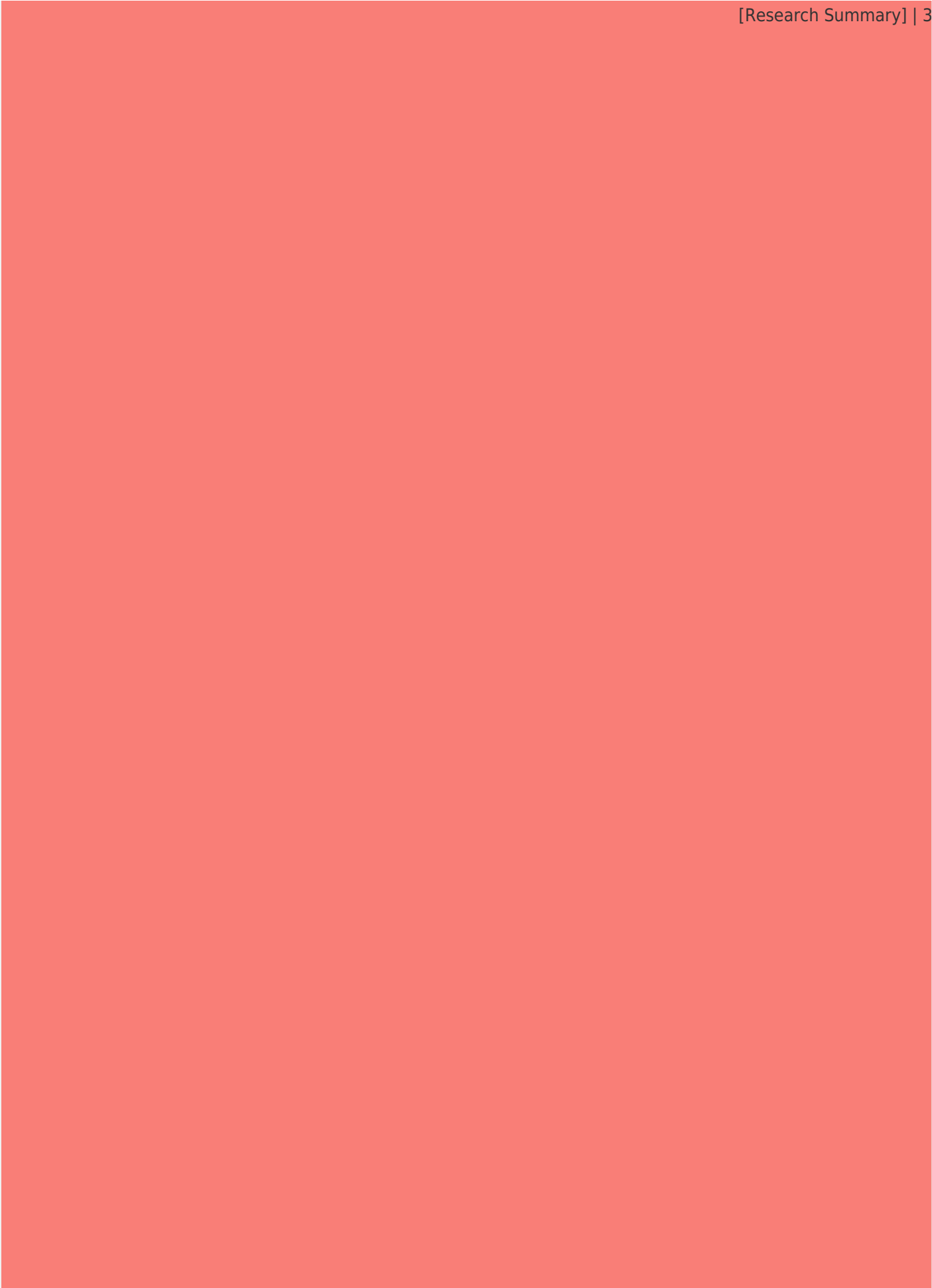
- [1] M. Sharma, D. Mishra, and J. Kumar, *First-Principles Study of the Structural and Electronic Properties of Bulk ZnS and Small ZnSn Nanoclusters in the Framework of the DFT+U method*, Physical Review 100, 045151 (2019).

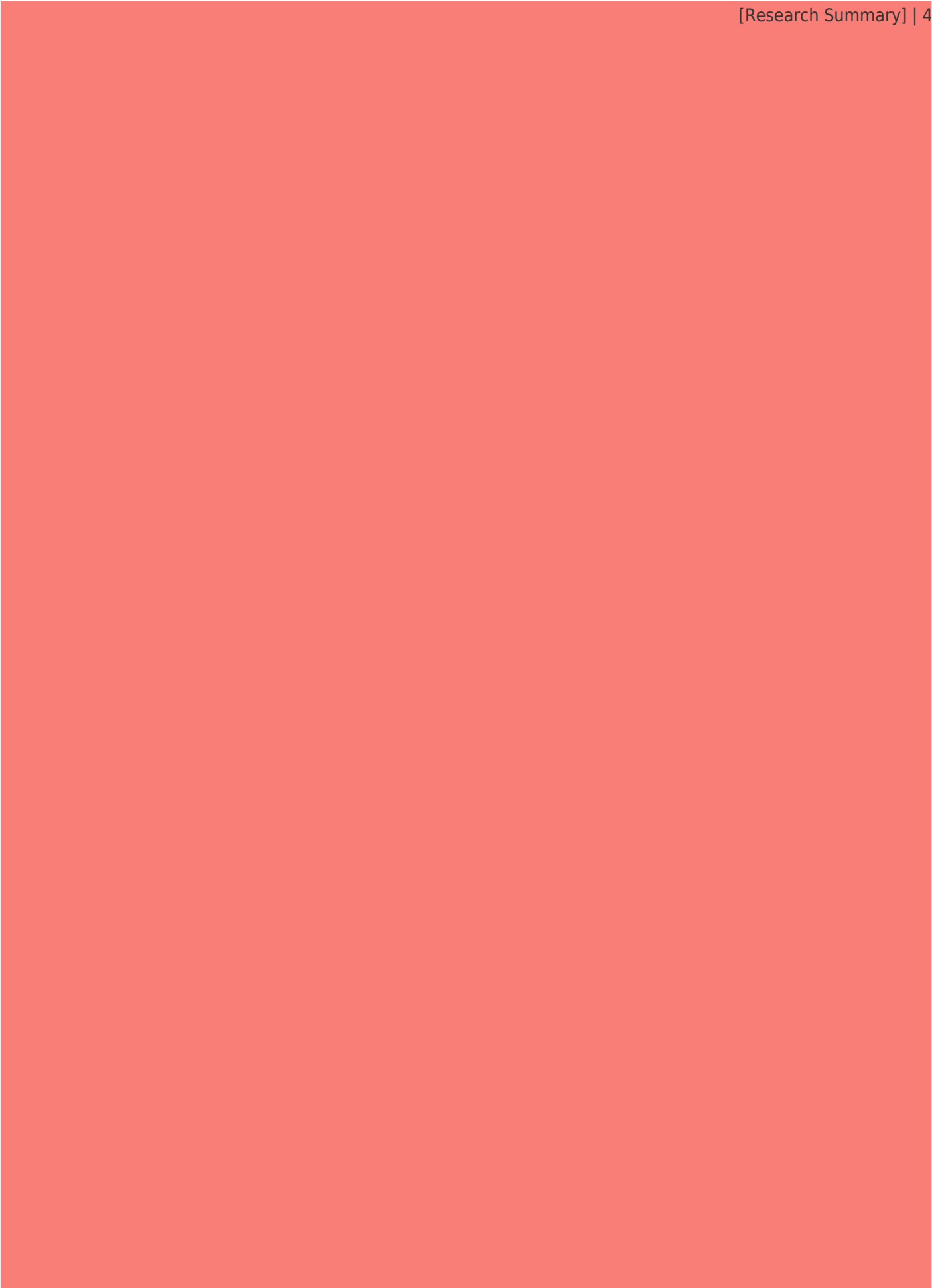


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