# Cover Letter

**Title**:
**Computational Structural, Electronic and Optical Properties of the Palmitic Acid in its C Form**

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We are pleased to submit our manuscript entitled for consideration to be published in Journal of Molecular Modeling.

IIn this manuscript, we report a theoretical study of the structural, electronic, and optical properties of palmitic acid crystal in its C form under DFT calculations level. We have found that the electronic bandstructure reveals an indirect gap of 3.713eV as the main bandgap, besides secondary bandgaps, around 4.175eV and 4.172eV, both indirect bandgaps. Our calculations revealed that effective masses of electrons and holes are anisotropic. On the contrary, optical absorption presents an isotropic behave in the interval from 5 to 25eV along with the (100), (010), and ( 601) directions. Already the dielectric function shows a weak anisotropy in the 5 to 10eV energy range along with the (001) and (101) directions. We conclude that palmitic acid structure behaves like a wide bandgap semiconductor, which points to potential applications in optoelectronic devices.

Based on the above, we believe this manuscript is appropriate for publication by the Journal of Molecular Modeling. Fatty acids like palmitic acid have potential applications in medicine, pharmaceuticals, cosmetics technology, foods, and fuel, besides semiconducting behavior, which provides great potential for industrial application. Lastly, no conflicts of interest exist in the submission of this manuscript. We appreciate your consideration of our manuscript, and we look forward to receiving comments from the reviewers.

Sincerely,

The authors.