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Structural and electronic properties of the organic semiconductor ZnPc

The structural and electronic properties of zinc phthalocyanine (ZnPc) monolayer were investigated using first-principles calculations. The calculated bond lengths and bond angles were found to be in good agreement with the previous works. The spin-polarized density of state (DOS) for ZnPc monolayer was presented. Furthermore, the effects of Sn intercalation on structural and electronic properties of ZnPc monolayer were also investigated. The change of bond lengths and bond angles nearby the intercalated Sn atom were analyzed. It was found that the obtained DOS is significantly changed by the intercalated Sn atom. The details of these behaviors were presented and discussed.

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