Theoretical Investigation on a New Two-dimensional Carbon Allotrope: Application in Optoelectronics and Photocatalysis

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The search for new carbon allotropes using theoretical approaches is an important subject in the field of computational materials science. Carbon exist in many allotropic forms across dimensions due to its ability to form sp, sp^2, sp^3, $sp+sp^2$ and sp^2+sp^3 -hybridized chemical bonds with itself. As a consequence, it reveals some interesting chemical, mechanical, electronic and optoelectronic properties. With advances of synthetic tools and simulation approach, a variety of novel carbon allotropes have already been realized experimentally or predicted by means of theoretically approach. In this presentation, we will discuss our simulation results of two-dimensional carbon allotropes for photocatalysis [1] and optoelectronic applications.

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References

[1] Babu Ram and Hiroshi Mizuseki, submitted