Discrete Geometric Analysis and Carbon Structures

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Discrete geometric analysis is a field that studies variational problems, eigenvalue problems, and geometry on graphs. We have conducted geometric research on sp^2 carbon structures, such as fullerenes, using the standard realization of topological crystals¹ based on variational problems on graphs.

In our study, we considered the sp^2 carbon structure as a trivalent discrete surface in three-dimensional Euclidean space and investigated its geometry². Furthermore, by using the standard realization of periodic graphs, we proposed a stable negatively curved carbon structure³.

The curvature of trivalent discrete surfaces is considered to be closely related to the physical properties of carbon structures. As an example, we demonstrated that the single nitrogen atom doping energy of 5-7 graphene is closely related to the rate of change in Gauss curvature before and after doping⁴.



References

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