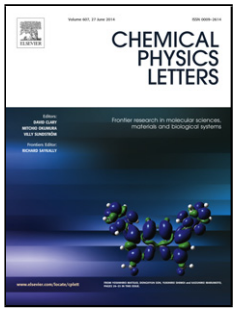

Title: Theoretical studies on the molecular structure, conformational preferences, topological and vibrational analysis of allicin

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Highlights

- The weak hydrogen bond S-O…H stabilizes the structure of allicin from the garlic *(Allium sativum L.)*.
- Car-Parrinello and path integrals molecular dynamics (CPMD/PIMD) of disulfide bond was performed.
- In the course of the CPMD, even in PIMD simulations fast proton transfer (FPT) within the hydrogen bond was not observed.
- The study of electronic structure of allicin that was performed in real space using topological analysis of electron localization function showed very similar nature of the S-S and S-O bonds.