

Abstract Submitted
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Diffusion of Various Molecules through Crystalline C₆₀ Solid and their Electronic and Vibrational Properties¹ YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — First-principles density functional theory is used to study the diffusion of various molecules including diatomic molecules, inert gas molecules, and small metal atoms, and so on, through the C₆₀ solid. For each case, the energy surface of a diffusion path is calculated while performing full geometry relaxation of the whole system. Such studies are performed while changing the concentrations of diffusing molecules. The effects of these molecules on the electronic properties of C₆₀ solid are also examined. Especially for diatomic molecules, such as H₂, N₂, and O₂, their frequency shifts are calculated relative to their corresponding counterparts.

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