개선된 반응표면모멘트법을 이용한 신뢰도 해석

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Reliability Analysis Using Enhanced Response Surface Moment Method (RSMM+)

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Key Words: Reliability Analysis(신뢰도 해석), Moment Method(모멘트법), DOE(실험계획법), Pearson System(피어슨 시스템), RSMM(반응표면모멘트법)

Abstract : The moment methods are powerful and simple methods for analyzing the reliability of a system response function. The full factorial moment method (FFMM) performs a reliability analysis by using a 3^n full factorial design of experiment (DOE) and the Pearson system. To overcome the inefficiency of FFMM, the response surface moment method (RSMM) is proposed, which is based on a response surface model. This paper proposes the enhanced RSMM (RSMM+) that modifies the procedure of selecting a cross product term in RSMM and adds a process of judging whether the response surface model can be established before performing an additional experiment. The proposed method is applied to several examples and gives better results in efficiency.

분자 첨점 조건을 고려한 토마스-페르미-아말디 방정식

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The grid-based Thomas-Fermi-Amaldi equation with molecular cusp conditions

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Key Words: DFT(밀도 범함수 이론), TFA(토마스-페르미-아말디), Cusp condition(첨점조건)

Abstract : First, the Thomas-Fermi-Amaldi (TFA) equation was formulated with a newly-derived condition to remove the singularities at the nuclei, coincided with the molecular cusp condition. Next, the collocation method was applied to the TFA equation using the grid-based density functional theory. In this paper, the electron densities for specific atoms (He, Be, Ne, Mg, Ar, Ca) and total energies for specific atoms (He, Ne, Ar, Kr, Xe, Rn) and molecules (H2, CH4) were found to agree with those from the Hartree-Fock method using the Pople basis set 6-31G. In addition, the computational expense to determine the electron density and its corresponding energy for a large scale structure, such as a carbon nanotube is shown to be much more efficient compared to the conventional Hartree-Fock method using the 6-31G Pople basis set.