

**STUDI INTERAKSI I₂ DAN IODOMETANA DENGAN KLUSTER Ag₁₀
DALAM SILIKA MORDENIT (Si-MOR): KAJIAN PERIODIK TIGA
DIMENSI TEORI FUNGSIONAL KERAPATAN**

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INTISARI

Kajian teoritis menggunakan teori fungsional kerapatan tiga dimensi untuk mempelajari interaksi kluster Ag dalam silika mordenit (Si-MOR) sebagai agen penangkap spesies iodin (I₂ dan iodometana) telah dilakukan. Penelitian ini bertujuan untuk mengkaji struktur yang terbentuk oleh kluster Ag₁₀ dalam *main channels* Si-MOR dan mengkaji interaksi yang terjadi antara spesies iodin dengan kluster Ag₁₀ di dalam *main channels* Si-MOR serta faktor-faktor yang memengaruhi interaksi tersebut. Hasil struktur teroptimasi, energi interaksi, dan densitas elektron diperoleh melalui metode perhitungan teori fungsional kerapatan tiga dimensi dengan fungsi korelasi-pertukaran PBESol.

Penelitian dilakukan melalui tiga tahap utama, validasi struktur kristal Si-MOR, penambahan kluster Ag₁₀ di dalam *main channels* Si-MOR, serta penambahan I₂ dan iodometana terhadap Si-MOR (kluster Ag₁₀) secara terpisah. Hasil validasi struktur kristal menunjukkan bahwa struktur kristal Si-MOR teroptimasi memiliki parameter kisi dengan nilai eror relatif sebesar 0,7 % terhadap parameter kisi dari data hasil eksperimental. Hasil ini menunjukkan bahwa optimasi kristal Si-MOR dengan metode DFT-PBESol telah berhasil tervalidasi. Hasil penambahan kluster Ag₁₀ di dalam *main channels* Si-MOR menunjukkan bahwa struktur Si-MOR (kluster Ag₁₀) dapat terbentuk secara stabil yang ditunjukkan melalui struktur Si-MOR yang terbentuk tidak mengalami *amorphization* dengan energi interaksi total sebesar -81,8 kkal/mol. Sementara itu, hasil penambahan I₂ dan iodometana terhadap Si-MOR (kluster Ag₁₀) secara terpisah memperlihatkan potensi keberhasilan kluster Ag₁₀ sebagai agen penangkap spesies iodin. Keberhasilan ini didasari pada tinjauan muatan parsial yang menunjukkan adanya interaksi Ag-I memiliki karakter ionik yang dikuatkan melalui hasil visualisasi densitas elektron dan energi interaksi antara Si-MOR (kluster Ag₁₀) dengan spesies iodin. Adapun energi interaksi total pada dua variasi uji diperoleh Si-MOR (kluster Ag₁₀ + I₂): -53,22 kkal/mol dan Si-MOR (kluster Ag₁₀ + ICH₃): -43,23 kkal/mol. Nilai kedua energi interaksi pada dua variasi tersebut menunjukkan bahwa sistem berada pada konfigurasi yang stabil serta berpotensi menjadi kandidat penangkap spesies iodin.

Kata kunci: agen penangkap spesies iodin, DFT, kluster Ag, silika mordenit

***INTERACTION STUDY OF I₂ AND IODOMETHANE WITH Ag₁₀ CLUSTERS
IN MORDENITE SILICA: A THREE-DIMENSIONAL PERIODIC STUDY OF
DENSITY FUNCTIONAL THEORY***

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ABSTRACT

Theoretical studies using three-dimensional density functional theory to study the effect of Ag clusters in silica mordenite (Si-MOR) as capture agents for iodine species (I₂ and iodomethane) have been carried out. This research aims to study the structures formed by Ag₁₀ clusters in the main channels of Si-MOR and the interactions that occur between iodine species on Ag₁₀ clusters in the main channels of Si-MOR as well as the factors that affect these interactions. The results of the optimized structure, interaction energy, and electron density were obtained through three-dimensional density functional theory calculations method with PBEsol exchange-correlation function.

The research was conducted through three main stages, validation of the Si-MOR crystal structure, addition of Ag₁₀ clusters in the main channels of Si-MOR, and addition of I₂ and iodomethane to Si-MOR (Ag₁₀ clusters) separately. The crystal structure validation results show that the optimized Si-MOR crystal structure has lattice parameters with a relative error value of 0.7 % against the lattice parameters from the experimental data. These results indicate that the optimization of Si-MOR crystals with the DFT-PBEsol method has been successfully validated. The results of the addition of Ag₁₀ clusters in the main channels of Si-MOR show that the structure of Si-MOR (Ag₁₀ clusters) can be formed stably as shown through the Si-MOR structure formed does not experience amorphization with a total interaction energy of -81.8 kcal/mol. Meanwhile, the results of the addition of I₂ and iodomethane to Si-MOR (Ag₁₀ cluster) separately showed the potential success of the Ag₁₀ cluster as an iodine species capture agent. This success is based on a partial charge review that shows the Ag-I interaction has an ionic character that is corroborated through the visualization of electron density and interaction energy between Si-MOR (Ag₁₀ cluster) and iodine species. The total interaction energy in the two test variations obtained by Si-MOR (Ag₁₀ + I₂ cluster): -53.22 kcal/mol and Si-MOR (Ag₁₀ + ICH₃ cluster): -43.23 kcal/mol. The values of both interaction energies in the two variations indicate that the system is in a stable configuration and has the potential to be a candidate for iodine species capture.

Keywords: Ag cluster, DFT, iodine species capture agents, silica mordenite