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Theoretical insight into the α, γ, δ-HMX molecules coexisting with β-HMX crystal at major facets by molecular dynamic simulations

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Molecular dynamics (MD) simulation was applied to research the effect of α, γ, δ-HMX molecules coexisting with β-HMX pure crystal at major facets on thermal stability, sensitivity, and mechanical properties of explosive before and after mixture. The binding energies, the maximum trigger bond length (LN-NO2), cohesive energy density (CED), and mechanical properties of mixture system and the corresponding pure crystal were got and compared. The results show that the β-HMX major crystal facets have great influence on the binding capacity of α, γ, δ-HMX molecules coexisting with β-HMX crystal and the binding energies of the mixture systems are commonly smaller than those of the corresponding pure one. The maximum trigger bond length doesn't change apparently after mixture, while the cohesive energy density decreases evidently, demonstrating that the sensitivity of the mixture systems increases. The mechanical properties decrease after mixture illustrating that the mechanical properties of the mixture systems are inferior to those of the pure crystals.