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RESEARCH PAPERS

二氧化钛(金红石)和六钛酸钾晶体的分子动力学模拟

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摘要 This paper presents the results of molecular dynamics (MD) simulation on the rutile titanium dioxide and potassium hexatitanate (K2O.6TiO2 or K2Ti6O13) crystal. The interaction of atoms is described by two-body central force interatomic potential, which includes Coulombic term, Gilbert-type repulsion term, van der Waals term and Morse-type potential. The optimized crystal structure of rutile TiO2 is in very good agreement with the experimental data in the literature. The present MD simulation also gives several physical properties, including volume thermal expansivity and elastic bulk modulus.

关键词 molecular dynamics molecular simulation titanium dioxide rutile potassium hexatitanate

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Molecular Dynamics Simulation of Rutile TiO_2 and Potassium Hexatitanate ($K_2Ti_6O_{13}$) Crystal

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Abstract This paper presents the results of molecular dynamics (MD) simulation on the rutile titanium dioxide and potassium hexatitanate (K2O.6TiO2 or K2Ti6O13) crystal. The interaction of atoms is described by two-body central force interatomic potential, which includes Coulombic term, Gilbert-type repulsion term, van der Waals term and Morse-type potential. The optimized crystal structure of rutile TiO2 is in very good agreement with the experimental data in the literature. The present MD simulation also gives several physical properties, including volume thermal expansivity and elastic bulk modulus.

Key words molecular dynamics; molecular simulation; titanium dioxide; rutile; potassium hexatitanate

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