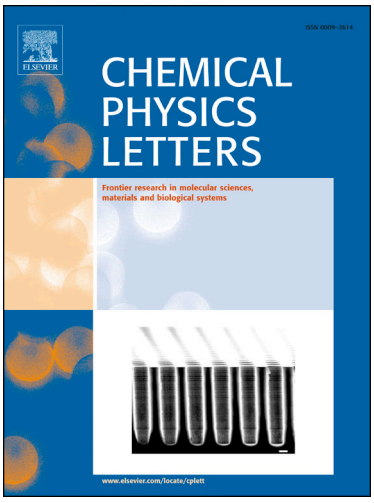

Research paper

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Gas Sensing Properties of Organotitanium Complex from First Principles Calculations and Molecular Dynamics Simulations

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Abstract

Gas sensing properties of C_2H_4Ti complex for monoxides and dioxides are studied using MP2/6-311++G** level and molecular dynamics (MD) simulations. Adsorption energies, geometric and electronic properties of an isolated and oxide adsorbed C_2H_4Ti complexes are studied. Density of state plot is used to study change in electronic properties of C_2H_4Ti complex after adsorption of oxides. Adsorption of all the oxide molecules is energetically favourable on C_2H_4Ti complex for entire temperature and pressure range considered. This is also confirmed using MD simulations. The C_2H_4Ti complex is suitable sensing material for monoxides and dioxides for a wide range of temperature and pressure.

Keyword: organotitanium complex; gas sensing; DOS; oxides; ab initio method; molecular dynamics simulation.

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Declarations of interest : None