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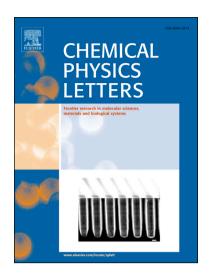
PII: S0009-2614(18)30499-8

DOI: https://doi.org/10.1016/j.cplett.2018.06.016

Reference: CPLETT 35715

To appear in: Chemical Physics Letters

Received Date: 6 March 2018 Revised Date: 8 June 2018 Accepted Date: 11 June 2018



Please cite this article as: N. Ingale, R. Konda, A. Chaudhari, Gas Sensing Properties of Organotitanium Complex from First Principles Calculations and Molecular Dynamics Simulations, *Chemical Physics Letters* (2018), doi: https://doi.org/10.1016/j.cplett.2018.06.016

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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 C₂H₄Ti 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 C₂H₄Ti

complexes are studied. Density of state plot is used to study change in electronic properties of

C₂H₄Ti complex after adsorption of oxides. Adsorption of all the oxide molecules is

energetically favourable on C₂H₄Ti complex for entire temperature and pressure range

considered. This is also confirmed using MD simulations. The C₂H₄Ti 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

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