

Poster 33

Structural, electronic and optical properties of spinel MgAl_2O_4 oxide

S. M. Hosseini

Department of Physics (Materials and Electroceramics Laboratory), Ferdowsi University of Mashhad, Iran

Abstract

The structural, the band structure, the total density of states, the dielectric function, the reflectivity, the refractive index and the loss function have been calculated for spinel MgAl_2O_4 oxide using density functional theory (DFT). The full potential linearized augmented plane wave (FL-LAPW) method was used with the generalized gradient approximation (GGA). The calculated results show a 5.2eV direct band gap along $\Gamma-\Gamma$ direction for this structure. Calculations of the optical spectra have been performed for the energy range 0-40eV. The high frequency dielectric constant, $\epsilon(\infty)$, of spinel MgAl_2O_4 oxide is equal to 3.112 and close to experimental value of 2.89. The excitonic transition associated with the fundamental absorption edge increases in the series from 6.27 to 10.19eV. It is shown that the material is transparent in the visible wavelengths and dispersion curve of refractive index is fairly flat in the long wavelength region and rises rapidly towards shorter wavelengths. The refractive index value is 1.774 at 800 nm near the visible region. The energy of volume plasmon, $\hbar\omega_p$, is assigned to the energy of the maximum peak of $\text{Im}[-\epsilon^{-1}(\omega)]$ is 27.66eV.

Delegate list

Computational Molecular Science 2008

David R Glowacki
University of Leeds
chmdrgl@leeds.ac.uk

Alex Hamilton
University of Bristol
chxah@bris.ac.uk

Richard Handel
University of Leicester
rjh52@le.ac.uk

Nicholas Handy
University of Cambridge
nchl@cam.ac.uk

Marlies Hankel
University of Queensland
m.hankel@uq.edu.au

Jean-Pierre Hansen
University of Cambridge
jph32@cam.ac.uk

Halvor Hansen
ETH Zürich
halvor@igc.phys.chem.ethz.ch

Judy Hart
University of Bristol
judy.hart@bris.ac.uk

Jeremy Harvey
University of Bristol
jeremy.harvey@bris.ac.uk

Martin Head-Gordon
University of California at
Berkeley
mhg@cchem.berkeley.edu

Richard Henchman
University of Manchester
henchman@manchester.ac.uk

Grant Hill
University of Cardiff
hilljg@cardiff.ac.uk

Quintin Hill
University of Southampton
quintin.hill@soton.ac.uk

Jonathan Hirst
University of Nottingham
jonathan.hirst@nottingham.ac.uk

James Hodge
PCCP, RSC Publishing
hodgej@rsc.org

Seyed M Hosseini Ferdowsi
University of Mashhad
sma_hosseini@yahoo.com

Sheeba Jem Irudayam
University of Manchester
sheeba.irudayam@postgrad.
manchester.ac.uk

Oksana Ismailova
University of Nottingham
oksana.ismailova@nottingham.
ac.uk

Robert Izsak
University of Cardiff
izsakr@cardiff.ac.uk

Maria Jaworska
University of Silesia
mj@ich.us.edu.pl

Jesús Jover Modrega
University of Bristol
jesus.jover@qi.ub.es

Johannes Kaestner
STFC Daresbury Laboratory
j.kaestner@dl.ac.uk

Steve Kaminski
TU Berlin
steve_kaminski@gmx.de

Thorsten Kampmann
Max Plank Institute for
Biophysical Chemistry
tkampma@gwdg.de

Tatyana Karabenchewa
University of Bristol
tatyana.karabenchewa@bris.ac.uk

Martin Karplus
Harvard University
marci@tammy.harvard.edu

Peter Knowles
University of Cardiff
knowlespj@cardiff.ac.uk

Rajat Kumar
Dav College Jalandhar
rajatkumar1069@yahoo.co.in

Anna-Pitschna E Kunz
ETH Zürich
pitschna@igc.phys.chem.ethz.ch

Narin Lawan
University of Bristol
chxnl@bris.ac.uk

Ruth Le Sueur
University of Durham
c.r.lesueur@dur.ac.uk

Dewi Lewis
University College London
d.w.lewis@ucl.ac.uk

Verónica Leyva Novoa Freie
Universität Berlin
voyoleno@chemie.fu-berlin.de

Miguel Machuqueiro
Instituto de Tecnologia Química e
Biológica
machuque@itqb.unl.pt

Fred Manby
University of Bristol
fred.manby@bris.ac.uk

David Manolopoulos
University of Oxford
mano@physchem.ox.ac.uk

Paulo Martel
University of Algarve
pmartel@ualg.pt

Andrew May
University of Cardiff
mayajl@cardiff.ac.uk

John McGeagh
University of Bristol
john.mcgeagh@bris.ac.uk

John McGrady
University of Glasgow
j.mcgrady@chem.gla.ac.uk

Simon McIntosh-Smith
ClearSpeed Technology plc
simon@clearspeed.com