

# **3rd Workshop on Theory, Modelling and Computational Methods for Semiconductors 2012**

**(TMCSIII)**

**Journal of Physics: Conference Series Volume 367**

**Leeds, United Kingdom  
18-20 January 2012**

**Editors:**

**Marco Califano  
Max Migliorato  
Matt Probert**

**ISBN: 978-1-62276-784-7  
ISSN: 1742-6588**

**Printed from e-media with permission by:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571



**Some format issues inherent in the e-media version may also appear in this print version.**

Copyright© (2012) by the Institute of Physics  
All rights reserved.

Printed by Curran Associates, Inc. (2013)

For permission requests, please contact the Institute of Physics  
at the address below.

Institute of Physics  
Dirac House, Temple Back  
Bristol BS1 6BE UK

Phone: 44 1 17 929 7481  
Fax: 44 1 17 920 0979

[techtracking@iop.org](mailto:techtracking@iop.org)

**Additional copies of this publication are available from:**

Curran Associates, Inc.  
57 Morehouse Lane  
Red Hook, NY 12571 USA  
Phone: 845-758-0400  
Fax: 845-758-2634  
Email: [curran@proceedings.com](mailto:curran@proceedings.com)  
Web: [www.proceedings.com](http://www.proceedings.com)

# TABLE OF CONTENTS

## AB INITIO

<b>012001 Optical Response of Extended Systems from Time-Dependent Hartree-Fock and Time-Dependent Density-Functional Theory</b> .....	1
<i>L Bernasconi, R Webster, S Tomic, N M Harrison</i>	
<b>012002 Linear-scaling Density Functional Theory Simulations of Polar Semiconductor Nanorods</b> .....	13
<i>N D M Hine, P W Avraam, P Tangney, P D Haynes</i>	
<b>012003 A Study of Atomic Orbital Basis Sets for Doped Silicon Nanowires</b> .....	23
<i>D Sharma, G Fagas</i>	
<b>012004 Density Functional Studies of the Defect-induced Electronic Structure Modifications in Bilayer Boronitrene</b> .....	29
<i>A M Ukpong, N Chetty</i>	

## NITRIDES

<b>012005 Non-linear Electro-elastic Coupling in Non-centrosymmetric Materials</b> .....	35
<i>J Even, L Pedesseau, C Hajlaoui, C Katan, J-M Jancu</i>	
<b>012006 Strain Dependence of Internal Displacement and Effective Charge in Wurtzite III-N Semiconductors</b> .....	41
<i>J Pal, G Tse, V Haxha, M A Migliorato, S Tomic</i>	

## QUANTUM NANOSTRUCTURES

<b>012007 Strain in Inhomogeneous InAs/GaAs Quantum Dot Structures</b> .....	47
<i>B Lassen, D Baretin, M Willatzen</i>	
<b>012008 Electron-LO Phonon and Electron-Photon Interactions Analogy in Semiconductor Quantum Dots</b> .....	52
<i>N Prodanovic, Z Ikonc, D Indjin, P Harrison</i>	
<b>012009 Photon Absorption in Periodically Regimented Nanostructures</b> .....	56
<i>A Luque-Rodríguez, F M Gómez-Campos, S Rodríguez-Bolívar</i>	
<b>012010 Accurate Light Scattering for Non Spherical Particles from Mie-type Theory</b> .....	60
<i>B Hourahine, K Holms, F Papoff</i>	

## DEVICES

<b>012011 Intersubband Thermophotovoltaics</b> .....	66
<i>M F Pereira</i>	
<b>012012 Compliant Energy and Momentum Conservation in NEGF Simulation of Electron-Phonon Scattering in Semiconductor Nano-wire Transistors</b> .....	71
<i>J R Barker, A Martinez, M Aldegunde</i>	
<b>012013 Noise Analysis of Gate Electrode Work Function Engineered Recessed Channel (GEWE-RC) MOSFET</b> .....	75
<i>A Agarwala, R Chaujar</i>	

## NANOSCALE SCIENCE AND DESIGN

<b>012014 Optoelectronic Properties of InAs/GaSb Superlattices with Asymmetric Interfaces</b> .....	83
<i>E Machowska-Podsiadlo, S Sujecki, T Benson, A Jasik, M Bugajski, K Pierscinski</i>	
<b>012015 Empirical Interatomic Potential for the Mechanical, Vibrational and Thermodynamic Properties of Semiconductors</b> .....	87
<i>U Monteverde, M A Migliorato, D Powell</i>	
<b>Author Index</b>	