

Nanotechnology  
Science and Technology

**Computer  
Investigation of  
the Stability and  
Structure of Si and  
SiO<sub>2</sub> Nanoparticles**

A. Y. Galashev  
V. A. Polukhin

NOVA

**NANOTECHNOLOGY SCIENCE AND TECHNOLOGY**

**COMPUTER INVESTIGATION OF  
THE STABILITY AND STRUCTURE  
OF SI AND SiO<sub>2</sub> NANOPARTICLES**

NANOTECHNOLOGY SCIENCE AND TECHNOLOGY

**COMPUTER INVESTIGATION OF  
THE STABILITY AND STRUCTURE  
OF SI AND SiO<sub>2</sub> NANOPARTICLES**

**A. Y. GALASHEV  
AND  
V. A. POLUKHIN**



**Nova Science Publishers, Inc.**

*New York*

Copyright © 2012 by Nova Science Publishers, Inc.

**All rights reserved.** No part of this book may be reproduced, stored in a retrieval system or transmitted in any form or by any means: electronic, electrostatic, magnetic, tape, mechanical photocopying, recording or otherwise without the written permission of the Publisher.

For permission to use material from this book please contact us:

Telephone 631-231-7269; Fax 631-231-8175

Web Site: <http://www.novapublishers.com>

### **NOTICE TO THE READER**

The Publisher has taken reasonable care in the preparation of this book, but makes no expressed or implied warranty of any kind and assumes no responsibility for any errors or omissions. No liability is assumed for incidental or consequential damages in connection with or arising out of information contained in this book. The Publisher shall not be liable for any special, consequential, or exemplary damages resulting, in whole or in part, from the readers' use of, or reliance upon, this material. Any parts of this book based on government reports are so indicated and copyright is claimed for those parts to the extent applicable to compilations of such works.

Independent verification should be sought for any data, advice or recommendations contained in this book. In addition, no responsibility is assumed by the publisher for any injury and/or damage to persons or property arising from any methods, products, instructions, ideas or otherwise contained in this publication.

This publication is designed to provide accurate and authoritative information with regard to the subject matter covered herein. It is sold with the clear understanding that the Publisher is not engaged in rendering legal or any other professional services. If legal or any other expert assistance is required, the services of a competent person should be sought. FROM A DECLARATION OF PARTICIPANTS JOINTLY ADOPTED BY A COMMITTEE OF THE AMERICAN BAR ASSOCIATION AND A COMMITTEE OF PUBLISHERS.

Additional color graphics may be available in the e-book version of this book.

### **Library of Congress Cataloging-in-Publication Data**

Galashev, Alexander Y.

Computer investigation of the stability and structure of Si and SiO<sub>2</sub> nanoparticles / authors, A.Y. Galashev, V.A. Polukhin.

p. cm.

Includes bibliographical references and index.

ISBN 978-1-61324-318-3 (softcover)

1. Nanoparticles--Computer simulation. 2. Silicon--Analysis--Data processing. I. Polukhin, V. A. (Valerii Anatol evich) II. Title.

TA418.9.N35G35 2011

620'.5--dc22

2011010114

*Published by Nova Science Publishers, Inc. †New York*

# CONTENTS

<b>Contents</b>		<b>v</b>
<b>Preface</b>		<b>vii</b>
<b>Abbreviations</b>		<b>xi</b>
<b>Chapter 1</b>	Introduction	<b>1</b>
<b>Chapter 2</b>	Molecular Dynamics Calculations	<b>9</b>
<b>Chapter 3</b>	Physicochemical Properties of Silicon Nanoparticles Containing 73 Atoms	<b>25</b>
<b>Chapter 4</b>	Molecular Dynamics Study of Hydrogenated Silicon Clusters at High Temperatures	<b>37</b>
<b>Chapter 5</b>	Simulation of Noncrystalline Silicon Nanoparticles	<b>57</b>
<b>Chapter 6</b>	Computer Simulation of Tension of Silicon Noncrystalline Nanoparticles	<b>67</b>
<b>Chapter 7</b>	Temperature Dependence of Physical Properties of Silicon Noncrystalline Nanoparticles	<b>81</b>
<b>Chapter 8</b>	Nucleation of Silicon Dioxide Nanoparticle in Closed Domain	<b>91</b>
<b>Chapter 9</b>	Computer Investigation of Structure of Porous SiO <sub>2</sub> Nanoparticle under Uniform Tension	<b>103</b>

<b>Chapter 10</b>	Concluding Remarks	<b>115</b>
<b>References</b>		<b>119</b>
<b>Index</b>		<b>127</b>