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01 March 2017 12:00

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Understanding molecular simulation; from algorithms to applications, 2d ed.

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Full text: ISBN: 0122673514

TITLE: Understanding molecular simulation; from algorithms to applications, 2d ed.

AUTHOR: Frenkel, Daan and Berend Smit.

PUBLISHER: Academic Press

PUBLISH DATE: 2002

PAGES: 638

PRICE: \$59.95

BINDING: Hardcover

SERIES: Computational science series; 1

LIBRARY OF CONGRESS CLASSIFICATION: QD461

REVIEW: This work for nonexperts involved in computer simulation explains the physics behind the techniques of molecular simulation in materials science, allowing those using simulation to choose appropriate techniques and improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use is demonstrated in case studies. This edition presents new material on areas such as transition path sampling and diffusive barrier crossing to simulate rare events, dissipative particle dynamics as a course-grained simulation technique, and parallel tempering for glassy Hamiltonians. Frenkel is affiliated with the FOM Institute for Atomic and Molecular Physics and teaches chemical engineering at the University of Amsterdam, The Netherlands. Smit teaches chemical engineering at the University of Amsterdam. (©2002 Book News, Inc., Portland, OR)

Publication title: Scitech Book News; Portland

Volume: 26

Issue: 2

Pages: n/a

Publication year: 2002

Publication date: Jun 2002

Year: 2002

Publisher: Ringgold Inc

Place of publication: Portland

Country of publication: United States

Publication subject: Bibliographies, Social Sciences: Comprehensive Works--Abstracting, Bibliographies, Statistics, Technology: Comprehensive Works--Abstracting, Bibliographies, Statistics

ISSN: 01966006

Source type: Magazines

Language of publication: English

Document type: Book Review

ProQuest document ID: 200105755

Document URL: <https://search.proquest.com/docview/200105755?accountid=14699>

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Last updated: 2010-06-06

Database: Health & Medical Collection

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