

คู่มือการใช้งาน

ACS IN
FOCUS

Understand the research, faster.



Booknet




ACS Publications
Most Trusted. Most Cited. Most Read.

รองรับการใช้งานภายใต้เครือข่ายของมหาวิทยาลัย

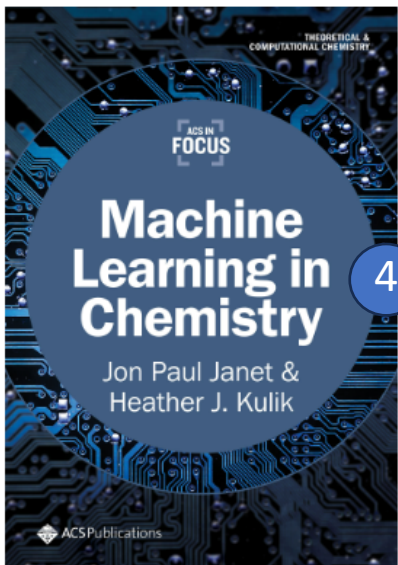
Platform access: <https://pubs.acs.org/series/infocus>

The screenshot shows the ACS Publications website interface. At the top, there is a navigation bar with the ACS logo and 'ACS Publications' text. Below this is a search bar with the placeholder text 'Search text, DOI, authors, etc.'. To the right of the search bar are icons for 'My Activity', 'Publications', and a menu icon. A green box highlights the text 'Access provided by ACCESS DUNIA SDN BHD' and 'Log In'. Below the navigation bar, the page is titled 'HOME PAGE'. There are two main sections: 'Newly Released & Coming Soon' and 'Most Popular'. Each section displays a row of book covers with titles and authors. The 'Newly Released & Coming Soon' section includes titles like 'Directed Evolution', 'Electrochemical Imaging', 'Protein Folding', 'Dynamics of a Liquid Droplet', 'Force-Responsive Networks', 'Theory of Block Polymer Self-Assembly', and 'Electron Paramagnetic Resonance Spectroscopy'. The 'Most Popular' section includes titles like 'Python for Chemists', 'Machine Learning in Chemistry', 'Photochemistry Essentials', 'Machine Learning in Materials Science', 'Metal-Organic Frameworks', 'Techniques in Electroanalytical Chemistry', and 'Machine Learning for Drug Discovery'. Numbered callouts 1-4 are placed over the page to highlight specific features: 1. Search bar, 2. 'Most Popular' section, 3. Access provided by ACCESS DUNIA SDN BHD, 4. User resources menu.



1. ช่องเมนูสืบค้น สามารถสืบค้นจาก keywords, ชื่อผู้แต่ง ฯลฯ
2. รายชื่อหนังสือแบ่งตามหัวข้อ สามารถเข้าใช้งานได้เฉพาะรายการหนังสือที่เป็นสมาชิกเท่านั้น
3. ชื่อสถาบันหากเข้าใช้งานถูกต้องจะแสดงชื่อของสถาบันหรือหน่วยงานของท่าน
4.  User resources, support แหล่งข้อมูลต่างๆ





Machine Learning in Chemistry

Author(s): Jon Paul Janet, Heather J. Kulik

Publication Date: May 29, 2020

Copyright © 2020 American Chemical Society

Subscribed

Cite This: *Machine Learning in Chemistry*, American Chemical Society, 2020. DOI: 10.1021/acs.infocus.7e4001

eISBN: 9780841299009

DOI: 10.1021/acs.infocus.7e4001

Subjects: Algorithms, Chemical engineering and industrial chemistry, Computational modeling, Machine learning, Neural networks, Theoretical and computational chemistry

Read Time: five to six hours

Collection: Inaugural

Publisher: American Chemical Society



Recent advances in machine learning or artificial intelligence for vision and natural language processing that have enabled the development of new technologies such as personal assistants or self-driving cars have brought machine learning and artificial intelligence to the forefront of popular culture. The accumulation of these algorithmic advances along with the increasing availability of large data sets and readily available high performance computing has played an important role in bringing machine learning applications to such a wide range of disciplines. Given the emphasis in the chemical sciences on the relationship between structure and function, whether in biochemistry or in materials chemistry, adoption of machine learning by chemists. *Machine Learning in Chemistry* focuses on the following to launch your understanding of this highly relevant topic:

+ Read more

Detailed Table of Contents

About the Series

Preface

1. Advancing Research through Machine Learning

2. Supervised Machine Learning for the Chemical Sciences

3. Linear Models, Kernels, and Trees

4. Representations of Atomistic Systems

5. Neural Networks and Learned Representations

6. Applying Machine Learning Models in Chemistry

Acronyms

Bibliography

Glossary

Nomenclature

Footnotes

Index

Author Info

Jon Paul Janet

Jon Paul Janet is a scientist with expertise in molecular machine learning. He is currently working on early stage drug discovery and previously developed machine-learning augmented virtual design strategies for inorganic complexes. He received a Ph.D. in

+ Read more

Search ACS for Jon Paul Janet

Heather J. Kulik

Professor Heather J. Kulik is an Associate Professor in the Department of Chemical Engineering at MIT. She received her B.E. in Chemical Engineering from the Cooper Union in 2004 and her Ph.D. from the Department of Materials Science and Engineering at

+ Read more

Search ACS for Heather J. Kulik



FAQs

Share Add to TOC



1. ชื่อเรื่อง ข้อมูลหนังสือชื่อผู้แต่ง

2. Read เพื่ออ่าน online

3. Table of contents สามารถเลือกอ่านแต่ละหัวข้อภายในเล่มได้

4. Cite This: กดเพื่อดาวน์โหลด Citation

5. Preview content

6. สามารถ Share, add to Mendeley, ฝังไฟล์ PDF (Fact sheet)

7. ข้อมูลที่เกี่ยวข้องกับผู้แต่ง สามารถสืบค้นงานเขียนของผู้แต่งได้



ACS INFOCUS ปัจจุบันมีทั้งหมด 5 Collections ห้องสมุดสามารถบอกรับสมาชิกเพิ่มแบบซื้อขาดได้ตาม Collections ดังนี้

1. INAUGURAL COLLECTION (10 titles, publishing between 5/20-6/21)
2. COLLECTION 1 (20 titles, publishing between 7/21-6/22)
3. COLLECTION 2 (20 titles, publishing between 7/22-6/23)
4. COLLECTION 3 (20 titles publishing between 7/23 - 6/24)
5. COLLECTION 4** (20 titles publishing between 7/24 - 6/25)

สามารถดาวน์โหลดรายการ แต่ละ collections ได้จาก

<https://pubs.acs.org/series/infocus> เลือกหัวข้อ [In Focus Title List](#)



Explore Institutional Access

[Buy Individual Copies](#)

[In Focus Title List](#)



ฝ่ายสนับสนุนฐานข้อมูลออนไลน์ บริษัทบุ๊คเน็ต จำกัด 02 - 769 3888