

**Age of MXenes, Volume 1.**  
**Fundamentals and Artificial Intelligence:**  
**Machine Learning Interventions**

The paper used in this publication meets the minimum requirements of American National Standard for Information Sciences—Permanence of Paper for Printed Library Materials, ANSI Z39.48-1984. | ISBN 9781713888482 (pod)

Copyright © 2023 American Chemical Society

All Rights Reserved. Reprographic copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Act is allowed for internal use only, provided that a per-chapter fee of \$40.25 plus \$0.75 per page is paid to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. Republication or reproduction for sale of pages in this book is permitted only under license from ACS. Direct these and other permission requests to ACS Copyright Office, Publications Division, 1155 16th Street, N.W., Washington, DC 20036.

The citation of trade names and/or names of manufacturers in this publication is not to be construed as an endorsement or as approval by ACS of the commercial products or services referenced herein; nor should the mere reference herein to any drawing, specification, chemical process, or other data be regarded as a license or as a conveyance of any right or permission to the holder, reader, or any other person or corporation, to manufacture, reproduce, use, or sell any patented invention or copyrighted work that may in any way be related thereto. Registered names, trademarks, etc., used in this publication, even without specific indication thereof, are not to be considered unprotected by law.

PRINTED IN THE UNITED STATES OF AMERICA

# Contents

|   |            |
|---|------------|
| <b>Preface</b> .....  | <b>ix</b>  |
| <b>1. 2D-Transition Metal Carbides and Nitrides: Materials for the Next Generation</b> .....                  | <b>1</b>   |
| Nilmani Kumar, Harpreet Singh, Madhu Khatri, and Neha Bhardwaj  |            |
| <b>2. Amalgamation of MXenes and Polymers for Multifunctional Nanocomposites</b> .....                        | <b>27</b>  |
| Yuqin Tian, Yanqi Ma, Xiaoling He, Li Zhang, Ying Chen, and Xinxin Sheng                                      |            |
| <b>3. MXene-Polyoxometalate Hybrid Materials: From Composites to Intercalates</b> .....                       | <b>55</b>  |
| Jun-Jie Zhu and Pedro Gomez-Romero  |            |
| <b>4. Emerging Trends in Advanced Synthesis and Properties: Mxenes as Super Materials..</b>                   | <b>71</b>  |
| Prakash Chandra   |            |
| <b>5. Progresses and Challenges in 2D MXenes: Synthesis, Intercalation/Delamination, and Storage</b> .....    | <b>101</b> |
| Nasima Khatun   |            |
| <b>6. Modeling and Simulation of Electrochemical, Thermoelectric, and Magnetic Properties of MXenes</b> ..... | <b>143</b> |
| Mandira Das, Himangshu Sekhar Sarmah, Himanshu Murari, and Subhradip Ghosh                                    |            |
| <b>7. Electrochemical CO<sub>2</sub> Conversion via MXenes: A DFT Perspective</b> .....                       | <b>169</b> |
| B. Moses Abraham, M. V. Jyothirmai, and Jayant K. Singh   |            |
| <b>8. MXenes: Synthetic Approaches and Sensing Advances</b> .....   | <b>185</b> |
| Dharaben J. Joshi, Naved I. Malek, and Suresh Kumar Kailasa   |            |
| <b>9. Biosensing Frontiers: MXenes and Their Composites</b> .....   | <b>213</b> |
| Rahul Pillai, Ramdas Balan, Derry Holaday, and Jandas Ponnath Janardhanan                                     |            |
| <b>10. Dimensionality-Dependent Synthesis and Photocatalytic MXenes</b> .....                                 | <b>237</b> |
| Abhinav Kapur, Navneet Kaur, and Ganga Ram Chaudhary  |            |
| <b>Editors' Biographies</b> .....   | <b>263</b> |

## Indexes

|                            |            |
|----------------------------|------------|
| <b>Author Index</b> .....  | <b>267</b> |
| <b>Subject Index</b> ..... | <b>269</b> |