

Contents

Preface — V

List of contributors — IX

Robert Black, Isaac Tamblyn

1 An overview of accelerated materials discovery — 1

Samira Siahrostami, Stanislav R. Stoyanov, Sergey Gusarov, Ian D. Gates,
Mohammadreza Karamad

2 Artificial intelligence for catalysis — 27

Steven B. Torrisi, John M. Gregoire, Junko Yano, Matthew R. Carbone,
Carla P. Gomes, Linda Hung, Santosh K. Suram

3 Artificial intelligence for materials spectroscopy — 65

Benjamin P. MacLeod, Fraser G. L. Parlane, Amanda K. Brown, Jason E. Hein,
Curtis P. Berlinguette

4 Flexible automation for self-driving laboratories — 105

John Dagdelen, Alex Dunn

5 Algorithms for materials discovery — 123

Gustavo Guzman

6 Industrial materials informatics — 165

About the editor — 201

Index — 203